Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:49 PM GMT

PDB ID	:	4YZF
Title	:	Crystal structure of the anion exchanger domain of human erythrocyte Band 3
Authors	:	Alguel, Y.; Arakawa, T.; Yugiri, T.K.; Iwanari, H.; Hatae, H.; Iwata, M.; Abe, Y.; Hino, T.; Suno, C.I.; Kuma, H.; Kang, D.; Murata, T.; Hamakubo, T.; Cameron, A.D.; Kobayashi, T.; Hamasaki, N.; Iwata, S.
Deposited on	:	2015-03-25
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

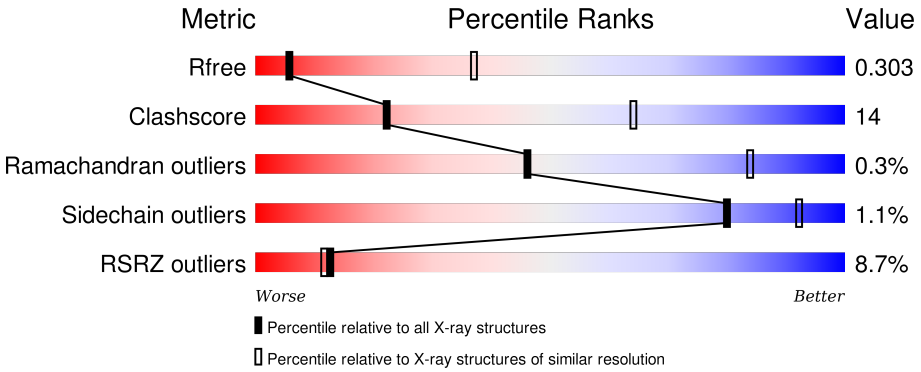
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	911	% 32% 19% • 48%
1	B	911	3% 32% 20% 48%
1	C	911	% 32% 20% 48%
1	D	911	3% 32% 20% 48%
2	E	223	10% 76% 22% •

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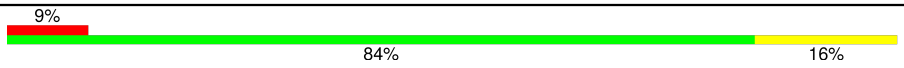
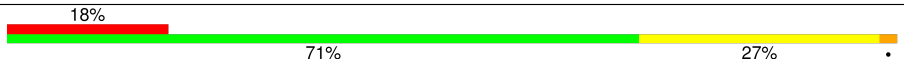
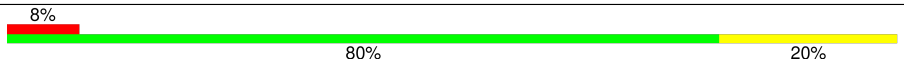
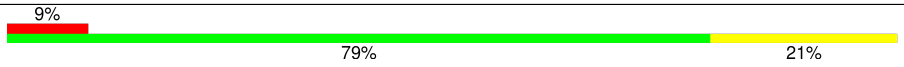
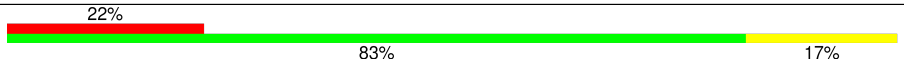
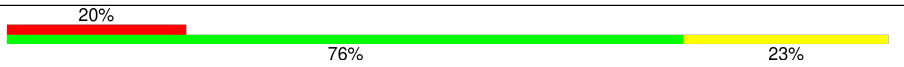
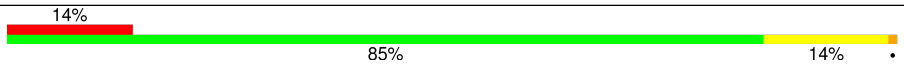
Mol	Chain	Length	Quality of chain
2	G	223	
2	I	223	
2	K	223	
3	F	218	
3	H	218	
3	J	218	
3	L	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28724 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	B	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	C	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			
1	D	475	Total	C	N	O	S	0	0	0
			3769	2535	598	619	17			

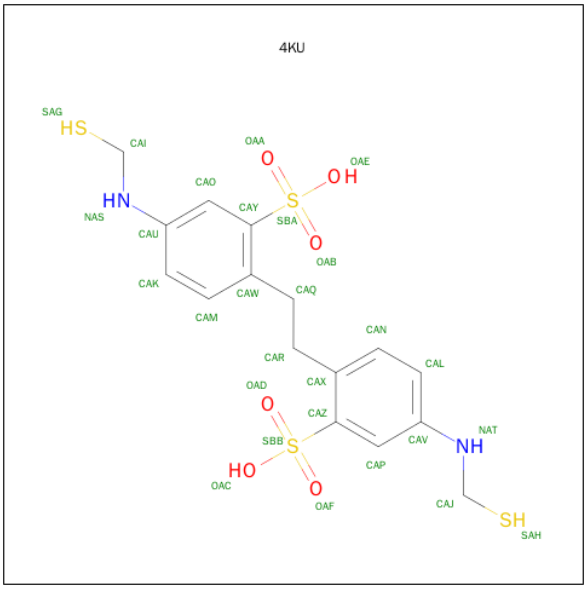
- Molecule 2 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	G	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	I	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			
2	K	223	Total	C	N	O	S	0	0	0
			1690	1077	274	334	5			

- Molecule 3 is a protein called FAB fragment of Immunoglobulin (IgG) molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	H	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	J	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			
3	L	218	Total	C	N	O	S	0	0	0
			1694	1055	285	346	8			

- Molecule 4 is 2,2'-ethane-1,2-diylbis{5-[(sulfanylmethyl)amino]benzenesulfonic acid} (three-letter code: 4KU) (formula: $C_{16}H_{20}N_2O_6S_4$).



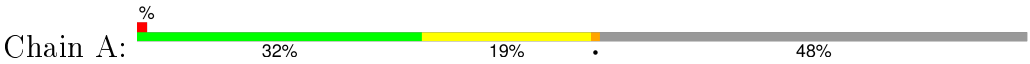
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	B	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	C	1	Total	C	N	O	S	0	0
			28	16	2	6	4		
4	D	1	Total	C	N	O	S	0	0
			28	16	2	6	4		

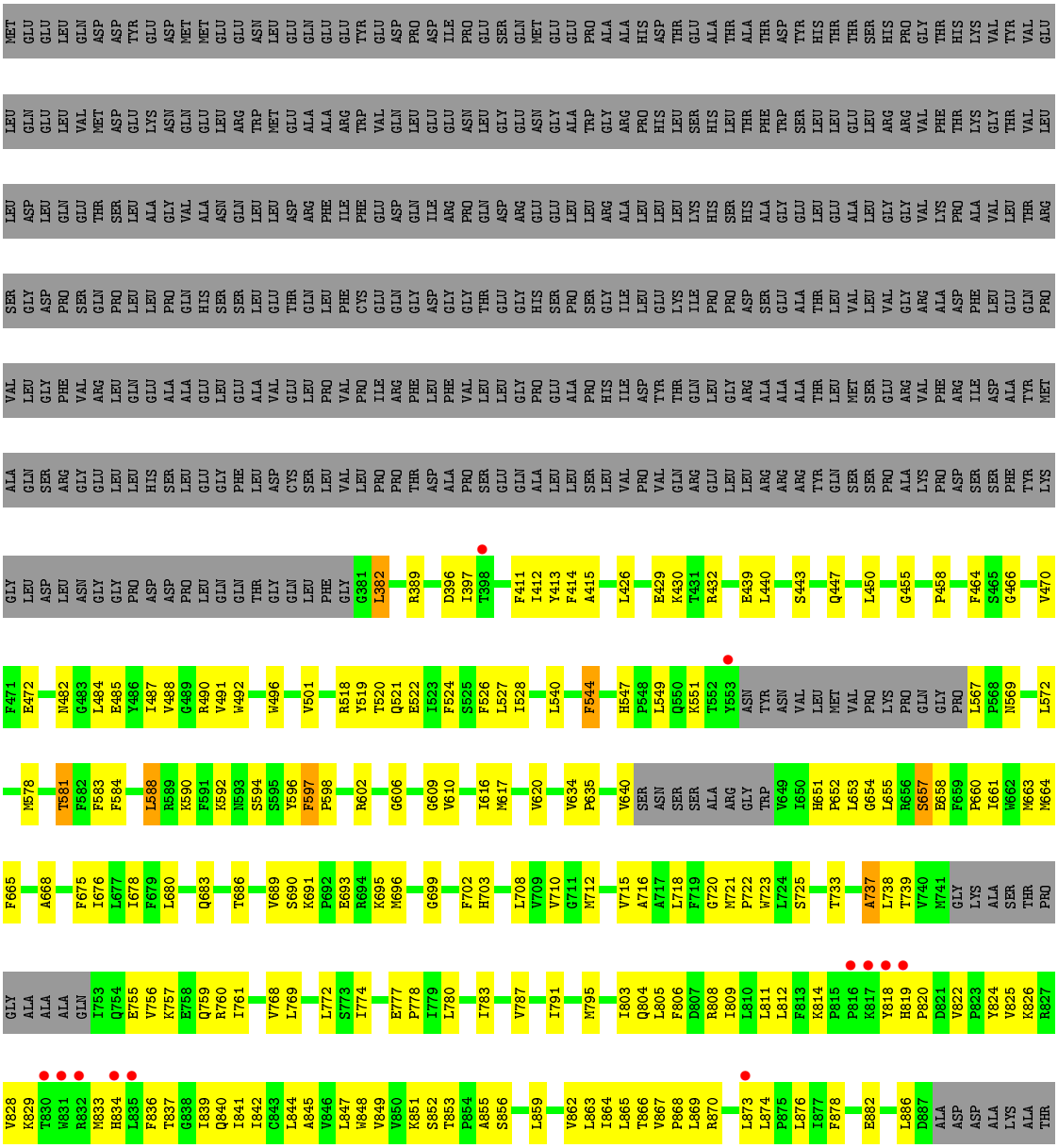
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Band 3 anion transport protein

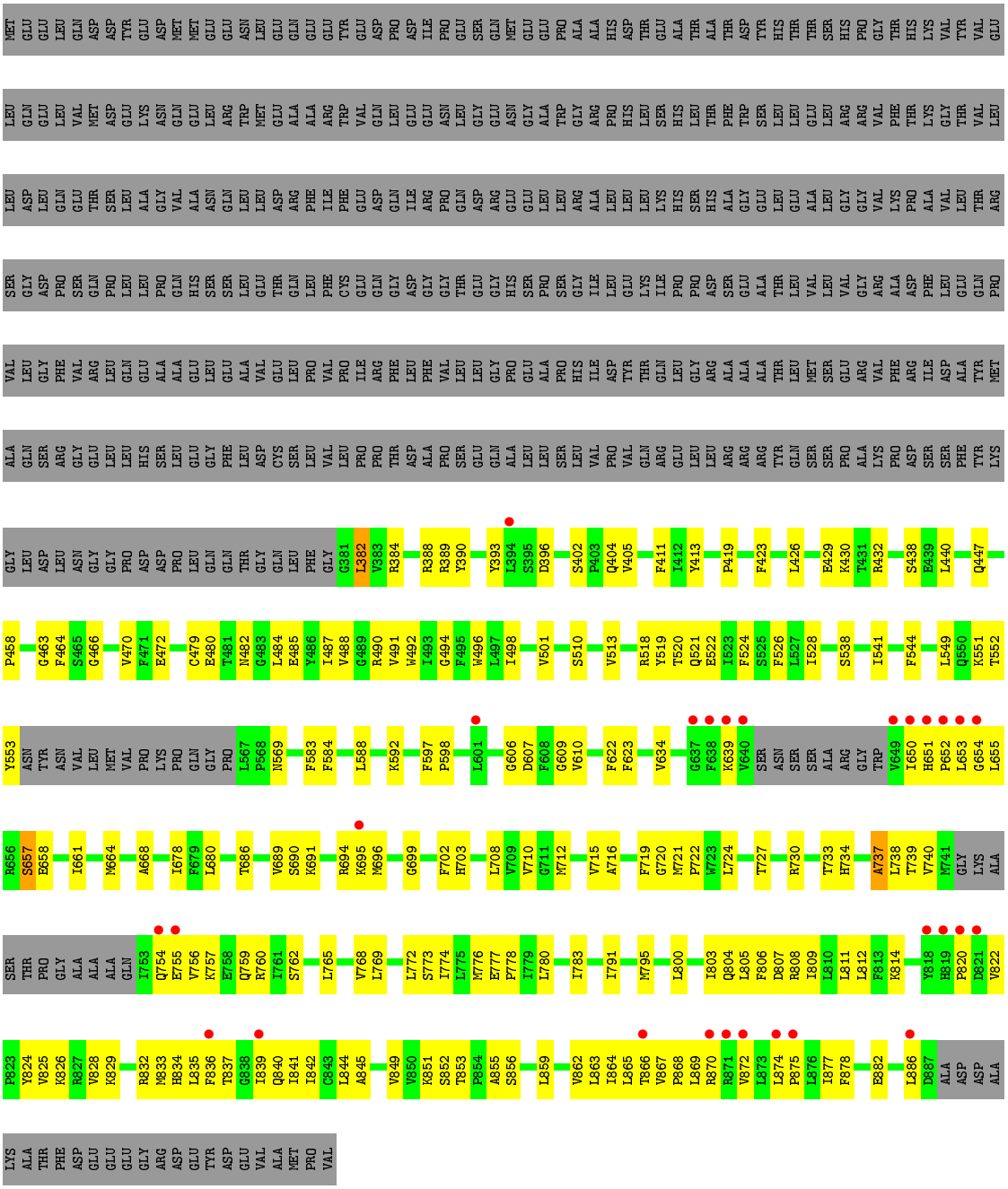
Chain A:





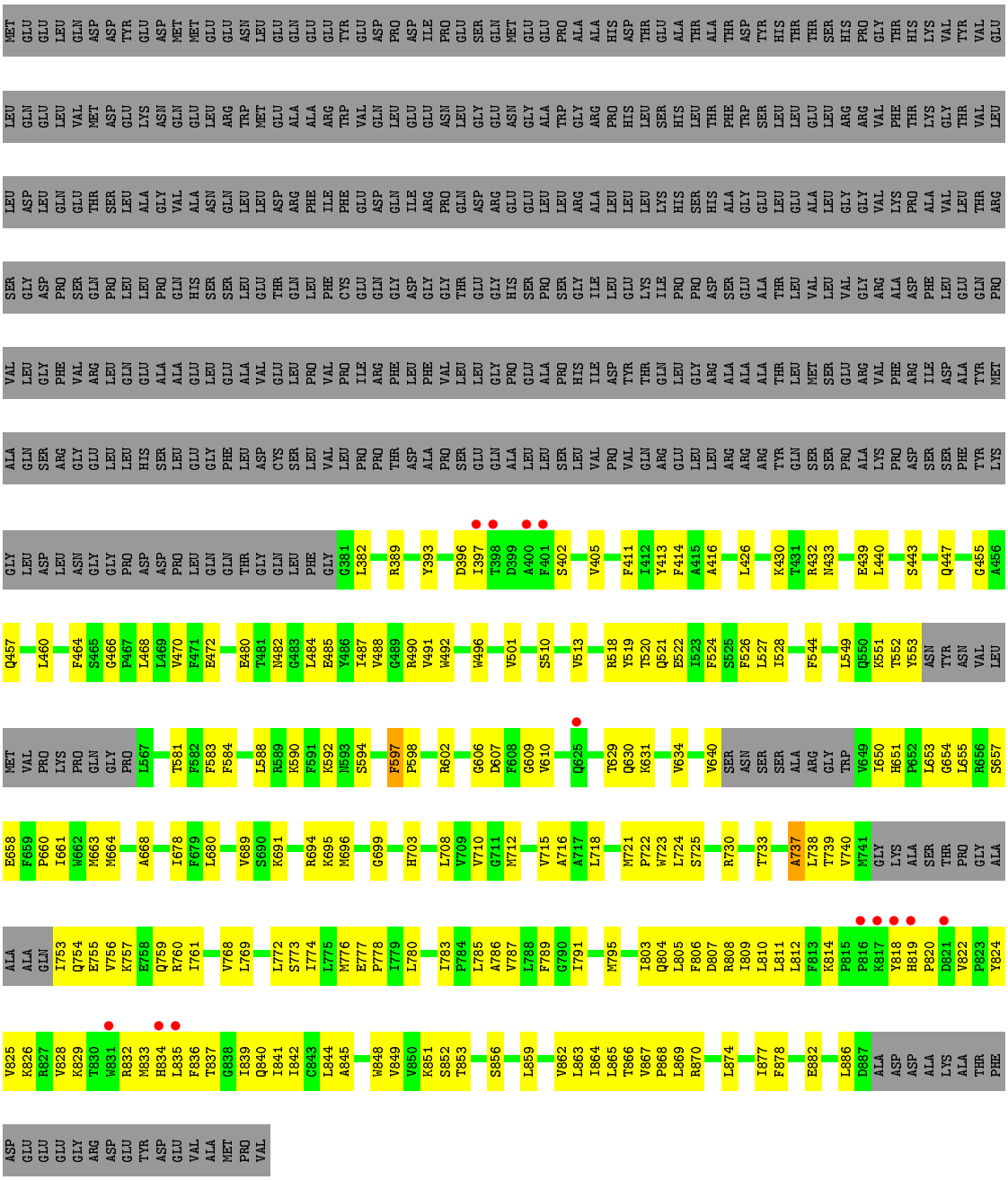
• Molecule 1: Band 3 anion transport protein

Chain B:



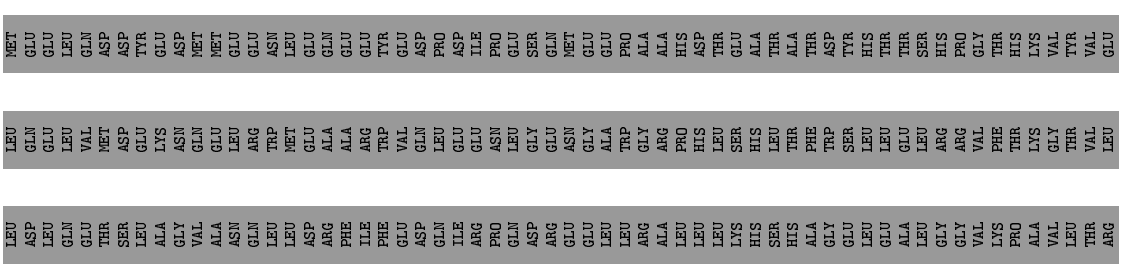
• Molecule 1: Band 3 anion transport protein

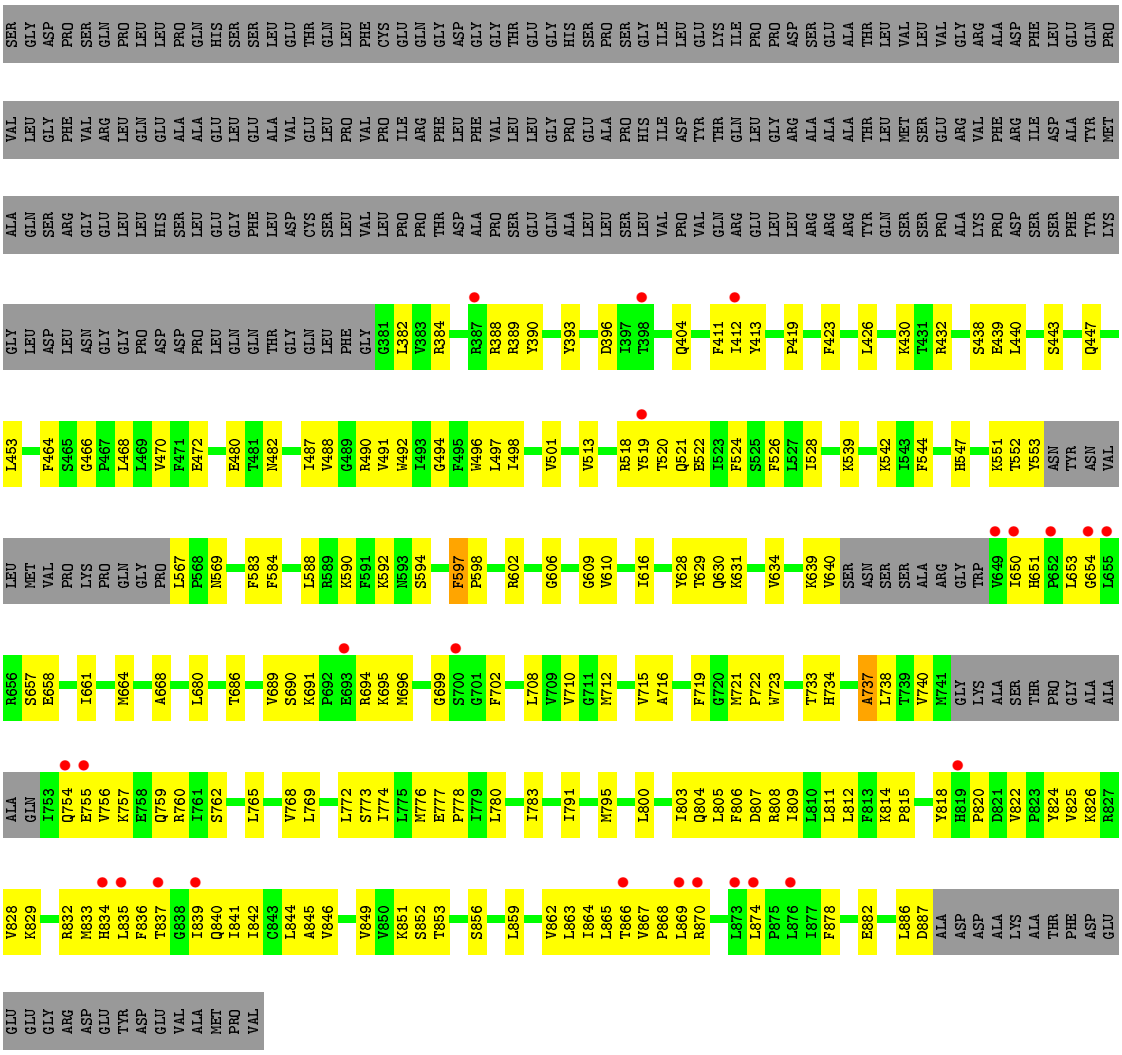
Chain C:



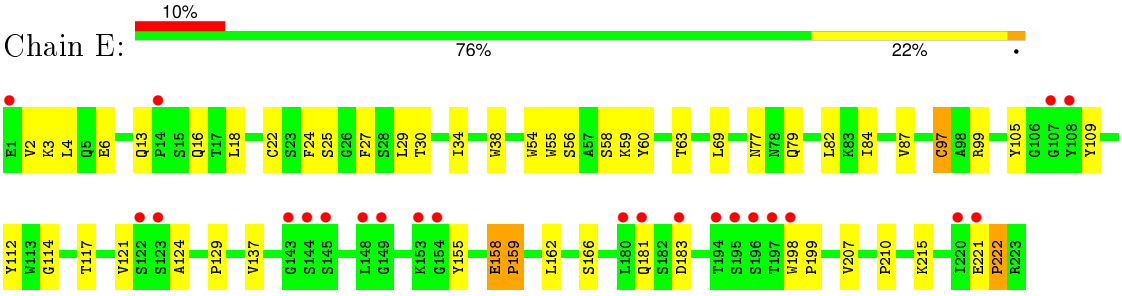
• Molecule 1: Band 3 anion transport protein

Chain D:

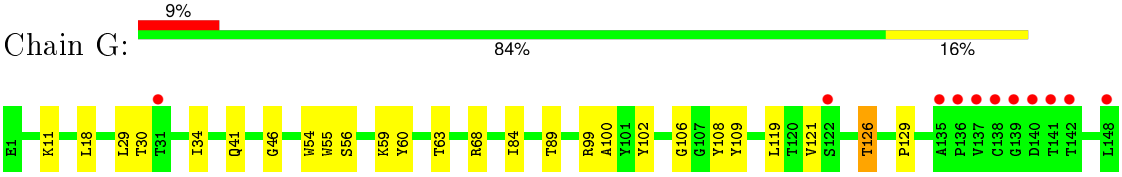


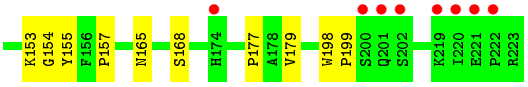


• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule



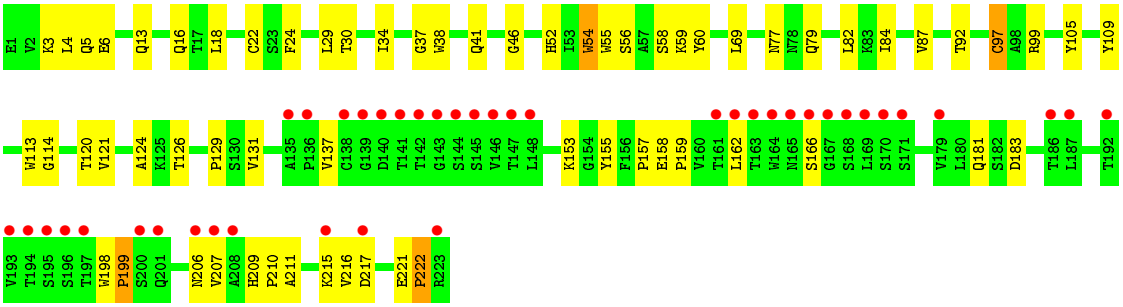
• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule





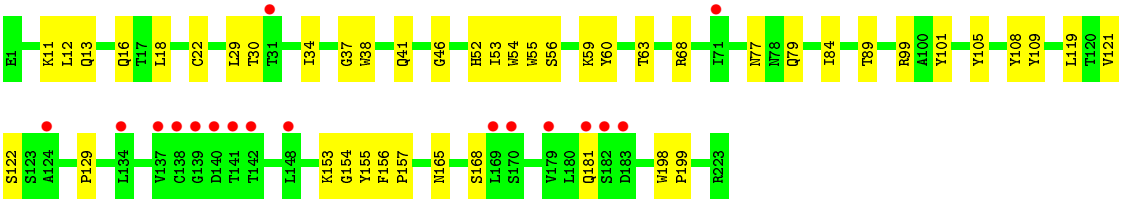
• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule

Chain I:



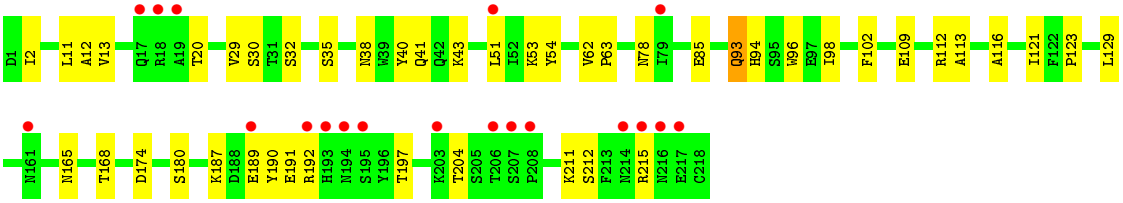
• Molecule 2: FAB fragment of Immunoglobulin (IgG) molecule

Chain K:



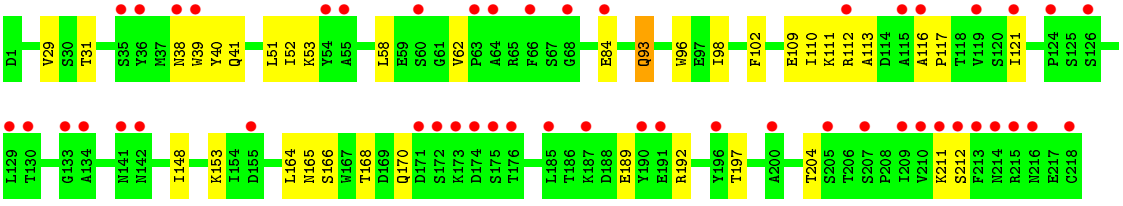
• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain F:



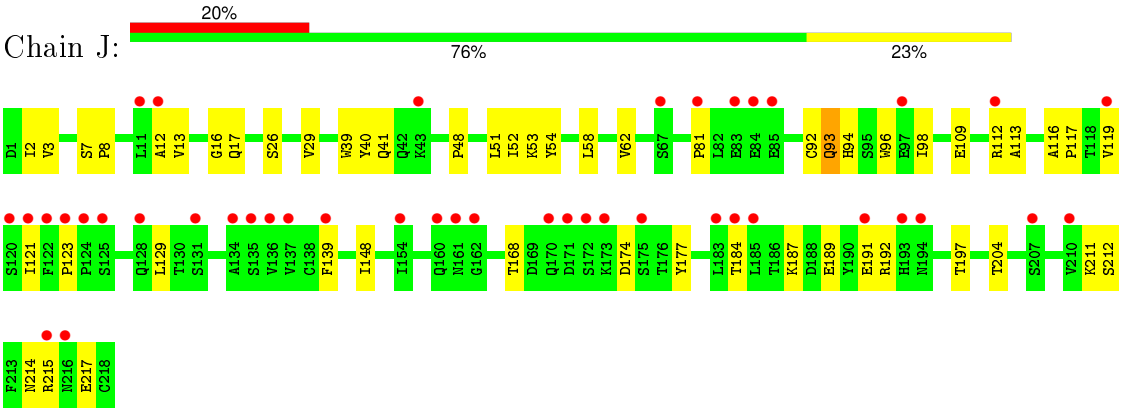
• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain H:



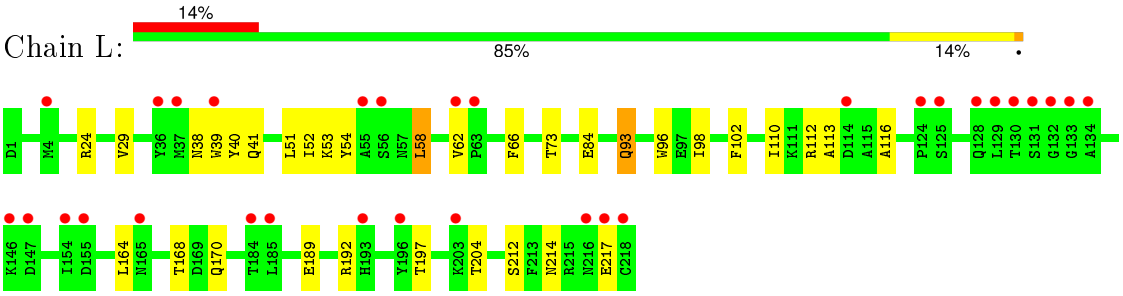
• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain J:



• Molecule 3: FAB fragment of Immunoglobulin (IgG) molecule

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.82Å 171.96Å 271.70Å 90.00° 101.16° 90.00°	Depositor
Resolution (Å)	37.72 – 3.50 48.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (37.72-3.50) 94.7 (48.84-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.274 , 0.290 0.287 , 0.303	Depositor DCC
R_{free} test set	4133 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	115.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 67.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	5 of 82522 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	28724	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.75 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3662e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4KU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/3862	0.62	2/5246 (0.0%)
1	B	0.37	0/3862	0.59	2/5246 (0.0%)
1	C	0.40	0/3862	0.60	1/5246 (0.0%)
1	D	0.37	0/3862	0.57	1/5246 (0.0%)
2	E	0.48	0/1737	0.90	3/2377 (0.1%)
2	G	0.39	0/1737	0.67	1/2377 (0.0%)
2	I	0.43	0/1737	0.81	3/2377 (0.1%)
2	K	0.37	0/1737	0.66	1/2377 (0.0%)
3	F	0.44	0/1736	0.64	0/2360
3	H	0.37	0/1736	0.57	1/2360 (0.0%)
3	J	0.37	0/1736	0.60	0/2360
3	L	0.34	0/1736	0.55	0/2360
All	All	0.40	0/29340	0.64	15/39932 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	68	ARG	NE-CZ-NH1	-7.19	116.70	120.30
2	E	158	GLU	C-N-CD	-6.51	106.27	120.60
2	K	68	ARG	NE-CZ-NH1	-5.98	117.31	120.30
2	I	158	GLU	C-N-CD	-5.73	107.99	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	737	ALA	C-N-CA	5.63	135.79	121.70
2	I	215	LYS	N-CA-C	-5.62	95.81	111.00
1	C	737	ALA	C-N-CA	5.58	135.64	121.70
2	E	97	CYS	N-CA-C	-5.32	96.64	111.00
2	I	97	CYS	N-CA-C	-5.29	96.72	111.00
1	B	737	ALA	C-N-CA	5.26	134.84	121.70
1	D	737	ALA	C-N-CA	5.19	134.67	121.70
3	H	109	GLU	OE1-CD-OE2	-5.14	117.13	123.30
2	E	215	LYS	N-CA-C	-5.14	97.13	111.00
1	B	657	SER	C-N-CA	5.07	134.37	121.70
1	A	657	SER	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	111	LYS	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3769	0	3990	150	0
1	B	3769	0	3990	141	0
1	C	3769	0	3988	138	0
1	D	3769	0	3989	144	0
2	E	1690	0	1645	40	0
2	G	1690	0	1645	28	0
2	I	1690	0	1645	45	0
2	K	1690	0	1645	33	0
3	F	1694	0	1609	33	0
3	H	1694	0	1609	28	0
3	J	1694	0	1609	40	0
3	L	1694	0	1609	26	0
4	A	28	0	15	1	0
4	B	28	0	14	2	0
4	C	28	0	15	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	15	2	0
All	All	28724	0	29032	798	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:VAL:HG23	1:A:829:LYS:HG3	1.48	0.94
1:D:851:LYS:HE3	1:D:859:LEU:HD22	1.51	0.92
1:C:828:VAL:HG23	1:C:829:LYS:HG3	1.49	0.92
1:D:828:VAL:HG23	1:D:829:LYS:HG3	1.54	0.90
1:D:737:ALA:HB3	1:D:738:LEU:HB2	1.55	0.89
1:B:737:ALA:HB3	1:B:738:LEU:HB2	1.55	0.89
2:I:124:ALA:HB2	2:I:183:ASP:HB3	1.53	0.89
1:C:851:LYS:HE3	1:C:859:LEU:HD22	1.52	0.89
1:D:592:LYS:HB2	1:D:606:GLY:HA3	1.56	0.88
1:C:592:LYS:HB2	1:C:606:GLY:HA3	1.55	0.88
1:C:737:ALA:HB3	1:C:738:LEU:HB2	1.55	0.87
2:K:30:THR:HA	2:K:55:TRP:HD1	1.38	0.87
1:A:851:LYS:HE3	1:A:859:LEU:HD22	1.57	0.86
1:A:737:ALA:HB3	1:A:738:LEU:HB2	1.54	0.86
1:B:592:LYS:HB2	1:B:606:GLY:HA3	1.58	0.85
3:F:112:ARG:NH1	3:F:174:ASP:O	2.09	0.85
1:B:828:VAL:HG23	1:B:829:LYS:HG3	1.57	0.85
1:A:592:LYS:HB2	1:A:606:GLY:HA3	1.58	0.83
2:E:30:THR:HA	2:E:55:TRP:CD1	2.16	0.81
2:I:30:THR:HA	2:I:55:TRP:CD1	2.16	0.80
2:E:30:THR:HA	2:E:55:TRP:HD1	1.47	0.80
1:B:501:VAL:HG21	1:B:710:VAL:HB	1.64	0.79
2:G:30:THR:HA	2:G:55:TRP:HD1	1.47	0.79
1:D:501:VAL:HG21	1:D:710:VAL:HB	1.64	0.79
1:A:549:LEU:HD22	1:B:569:ASN:HD21	1.47	0.79
1:C:518:ARG:NH1	1:C:804:GLN:OE1	2.17	0.78
1:B:851:LYS:HE3	1:B:859:LEU:HD22	1.63	0.78
1:A:610:VAL:HG13	1:A:791:ILE:HD12	1.65	0.77
3:H:29:VAL:HG23	3:H:96:TRP:HB2	1.66	0.77
1:A:518:ARG:NH1	1:A:804:GLN:OE1	2.18	0.77
1:D:519:TYR:HD2	1:D:867:VAL:HG13	1.49	0.77
1:C:501:VAL:HG21	1:C:710:VAL:HB	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:ILE:HG12	1:C:841:ILE:HD11	1.66	0.76
1:C:829:LYS:HB3	1:C:833:MET:N	2.00	0.76
1:C:610:VAL:HG13	1:C:791:ILE:HD12	1.68	0.76
2:G:11:LYS:HE3	2:G:126:THR:HG23	1.67	0.76
3:H:41:GLN:HB2	3:H:51:LEU:HD11	1.66	0.75
1:A:389:ARG:NH1	1:A:699:GLY:O	2.19	0.75
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.68	0.75
1:C:389:ARG:NH1	1:C:699:GLY:O	2.21	0.74
2:E:124:ALA:HB2	2:E:183:ASP:HB3	1.68	0.74
1:B:389:ARG:NH1	1:B:699:GLY:O	2.20	0.74
1:A:501:VAL:HG21	1:A:710:VAL:HB	1.69	0.74
1:B:829:LYS:HB3	1:B:833:MET:N	2.03	0.74
2:K:30:THR:HA	2:K:55:TRP:CD1	2.22	0.73
1:D:829:LYS:HB3	1:D:833:MET:N	2.04	0.73
1:D:518:ARG:NH1	1:D:804:GLN:OE1	2.22	0.73
1:B:519:TYR:HD2	1:B:867:VAL:HG13	1.54	0.72
3:J:112:ARG:NH1	3:J:174:ASP:O	2.20	0.72
2:I:30:THR:HA	2:I:55:TRP:HD1	1.54	0.72
1:D:520:THR:OG1	1:D:521:GLN:N	2.23	0.71
1:A:680:LEU:HD21	1:A:863:LEU:HD23	1.72	0.71
1:B:829:LYS:HB3	1:B:833:MET:H	1.56	0.71
1:D:389:ARG:NH2	1:D:396:ASP:OD2	2.18	0.71
3:J:109:GLU:OE2	3:J:177:TYR:OH	2.06	0.70
1:C:680:LEU:HD21	1:C:863:LEU:HD23	1.72	0.70
1:D:610:VAL:HG13	1:D:791:ILE:HD12	1.72	0.70
3:L:29:VAL:HG23	3:L:96:TRP:HB2	1.72	0.70
1:C:829:LYS:HB3	1:C:833:MET:H	1.56	0.70
1:A:829:LYS:HB3	1:A:833:MET:N	2.05	0.70
1:D:389:ARG:NH1	1:D:699:GLY:O	2.25	0.70
2:G:30:THR:HA	2:G:55:TRP:CD1	2.26	0.70
2:G:165:ASN:O	2:G:168:SER:OG	2.09	0.70
1:C:488:VAL:HG21	1:C:654:GLY:HA2	1.74	0.69
1:A:851:LYS:HB2	1:A:859:LEU:HD13	1.74	0.69
3:J:112:ARG:HH12	3:J:174:ASP:HB2	1.58	0.69
1:C:522:GLU:OE1	1:C:805:LEU:N	2.22	0.69
1:C:812:LEU:HA	1:C:834:HIS:CE1	2.28	0.68
3:F:29:VAL:HG23	3:F:96:TRP:HB2	1.76	0.68
1:A:812:LEU:HA	1:A:834:HIS:CE1	2.28	0.68
1:A:522:GLU:OE1	1:A:805:LEU:N	2.23	0.68
2:E:13:GLN:HB2	2:E:16:GLN:CD	2.14	0.68
3:J:29:VAL:HG23	3:J:96:TRP:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:GLN:HG2	1:C:712:MET:HB3	1.74	0.68
1:B:520:THR:OG1	1:B:521:GLN:N	2.24	0.68
1:B:480:GLU:O	2:G:108:TYR:OH	2.09	0.68
1:A:829:LYS:HB3	1:A:833:MET:H	1.60	0.67
1:B:526:PHE:CD2	1:B:844:LEU:HD21	2.29	0.67
2:G:60:TYR:CD1	3:H:98:ILE:HG21	2.29	0.67
1:B:610:VAL:HG13	1:B:791:ILE:HD12	1.74	0.67
1:A:520:THR:HG22	1:A:867:VAL:HG11	1.75	0.67
1:D:708:LEU:O	1:D:712:MET:HG2	1.95	0.67
2:E:13:GLN:HB2	2:E:16:GLN:NE2	2.10	0.67
1:A:526:PHE:CD2	1:A:844:LEU:HD21	2.30	0.67
1:B:809:ILE:HG12	1:B:841:ILE:HD11	1.76	0.67
1:D:829:LYS:HB3	1:D:833:MET:H	1.59	0.66
1:D:809:ILE:HG12	1:D:841:ILE:HD11	1.77	0.66
3:H:197:THR:OG1	3:H:212:SER:OG	2.14	0.66
1:C:803:ILE:HG22	1:C:806:PHE:H	1.59	0.66
2:E:54:TRP:CH2	2:E:60:TYR:HD2	2.14	0.66
3:H:84:GLU:HA	3:H:110:ILE:HD11	1.75	0.66
3:J:189:GLU:HA	3:J:192:ARG:HG3	1.77	0.66
1:D:480:GLU:O	2:K:108:TYR:OH	2.10	0.66
1:C:526:PHE:CD2	1:C:844:LEU:HD21	2.31	0.66
3:J:197:THR:HG1	3:J:212:SER:HG	1.39	0.65
1:B:588:LEU:HD12	1:B:609:GLY:HA2	1.78	0.65
1:A:519:TYR:HD2	1:A:867:VAL:HG13	1.62	0.65
1:B:689:VAL:HG12	1:B:696:MET:HE1	1.79	0.65
3:L:197:THR:HG1	3:L:212:SER:HG	1.44	0.65
1:D:522:GLU:OE1	1:D:805:LEU:N	2.24	0.65
1:C:520:THR:OG1	1:C:521:GLN:N	2.28	0.65
1:A:447:GLN:HG2	1:A:712:MET:HB3	1.78	0.65
3:H:51:LEU:HA	3:H:62:VAL:HG21	1.79	0.64
2:I:129:PRO:HB3	2:I:155:TYR:HB3	1.79	0.64
1:A:488:VAL:HG21	1:A:654:GLY:HA2	1.79	0.64
1:C:708:LEU:O	1:C:712:MET:HG2	1.97	0.64
1:A:413:TYR:CD1	1:A:769:LEU:HB3	2.32	0.64
2:K:60:TYR:CD1	3:L:98:ILE:HG21	2.32	0.64
1:B:820:PRO:HD3	1:B:826:LYS:HD2	1.78	0.64
2:E:6:GLU:O	2:E:117:THR:HB	1.98	0.64
1:D:680:LEU:HD21	1:D:863:LEU:HD23	1.80	0.64
1:C:482:ASN:HB3	2:I:56:SER:OG	1.97	0.64
1:A:803:ILE:HG22	1:A:806:PHE:H	1.62	0.63
1:A:809:ILE:HG12	1:A:841:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:TYR:CD1	1:B:769:LEU:HB3	2.33	0.63
1:D:867:VAL:HB	1:D:868:PRO:HD3	1.80	0.63
1:D:832:ARG:HD3	1:D:835:LEU:HD12	1.80	0.63
3:J:40:TYR:HE2	3:J:93:GLN:HG2	1.64	0.63
1:B:806:PHE:HA	1:B:809:ILE:HD12	1.81	0.62
1:C:689:VAL:HG12	1:C:696:MET:HE1	1.80	0.62
1:B:488:VAL:HG21	1:B:654:GLY:HA2	1.80	0.62
1:C:658:GLU:HG2	2:I:59:LYS:CG	2.30	0.62
1:D:526:PHE:CD2	1:D:844:LEU:HD21	2.34	0.62
1:A:520:THR:OG1	1:A:521:GLN:N	2.31	0.62
2:I:34:ILE:HG23	2:I:99:ARG:HD2	1.81	0.62
1:A:492:TRP:CD2	1:A:664:MET:HB2	2.35	0.62
1:A:824:TYR:O	1:A:828:VAL:HG22	2.00	0.62
1:D:432:ARG:HG2	3:L:96:TRP:CZ3	2.35	0.62
1:B:867:VAL:HB	1:B:868:PRO:HD3	1.81	0.62
1:C:824:TYR:O	1:C:828:VAL:HG22	2.00	0.61
3:F:112:ARG:HH12	3:F:174:ASP:HB2	1.64	0.61
1:C:588:LEU:HD12	1:C:609:GLY:HA2	1.82	0.61
3:F:197:THR:OG1	3:F:212:SER:OG	2.17	0.61
1:D:811:LEU:HD22	1:D:826:LYS:HZ1	1.64	0.61
1:D:851:LYS:HA	1:D:856:SER:HB2	1.83	0.61
1:B:518:ARG:NH1	1:B:804:GLN:OE1	2.34	0.61
1:C:867:VAL:HB	1:C:868:PRO:HD3	1.82	0.61
1:C:519:TYR:HD2	1:C:867:VAL:HG13	1.66	0.61
1:C:413:TYR:CD1	1:C:769:LEU:HB3	2.36	0.61
1:A:820:PRO:HD3	1:A:826:LYS:HD2	1.83	0.61
1:B:447:GLN:HG2	1:B:712:MET:HB3	1.83	0.61
1:D:808:ARG:NH2	1:D:840:GLN:HG3	2.14	0.61
1:A:651:HIS:CD2	1:A:653:LEU:HB2	2.34	0.61
1:D:757:LYS:HB3	1:D:759:GLN:HE22	1.66	0.61
1:C:658:GLU:HG2	2:I:59:LYS:HG2	1.82	0.61
1:C:820:PRO:HD3	1:C:826:LYS:HD2	1.83	0.61
1:C:691:LYS:HE2	1:C:694:ARG:HE	1.64	0.60
1:C:484:LEU:HD13	1:C:663:MET:HG2	1.83	0.60
1:D:820:PRO:HD3	1:D:826:LYS:HD2	1.82	0.60
1:B:832:ARG:HD3	1:B:835:LEU:HD12	1.82	0.60
1:B:824:TYR:O	1:B:828:VAL:HG22	2.02	0.60
1:D:689:VAL:HG12	1:D:696:MET:HE1	1.82	0.60
1:D:824:TYR:O	1:D:828:VAL:HG22	2.02	0.60
1:C:780:LEU:HA	1:C:783:ILE:HD12	1.83	0.60
4:C:1000:4KU:H18	4:C:1000:4KU:SAH	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:851:LYS:HB2	1:C:859:LEU:HD13	1.84	0.60
1:B:836:PHE:CD2	1:B:886:LEU:HD13	2.37	0.60
1:A:716:ALA:HB1	1:A:721:MET:HB2	1.84	0.60
1:C:520:THR:HG22	1:C:867:VAL:HG11	1.84	0.60
1:C:716:ALA:HB1	1:C:721:MET:HB2	1.82	0.60
1:C:492:TRP:CE2	1:C:664:MET:HB2	2.37	0.60
2:I:198:TRP:CH2	2:I:222:PRO:HG3	2.38	0.59
3:H:189:GLU:HA	3:H:192:ARG:HG3	1.85	0.59
1:B:389:ARG:NH2	1:B:396:ASP:OD2	2.24	0.59
1:A:584:PHE:HE2	1:A:616:ILE:HG21	1.67	0.59
1:B:466:GLY:O	1:B:470:VAL:HG23	2.02	0.59
1:A:867:VAL:HB	1:A:868:PRO:HD3	1.84	0.59
1:C:492:TRP:CD2	1:C:664:MET:HB2	2.37	0.59
1:D:447:GLN:HG2	1:D:712:MET:HB3	1.84	0.59
4:A:1000:4KU:H18	4:A:1000:4KU:SAH	2.42	0.59
1:C:389:ARG:NH2	1:C:396:ASP:OD2	2.21	0.59
1:B:426:LEU:O	1:B:430:LYS:HG2	2.03	0.59
1:B:661:ILE:O	1:B:664:MET:HG2	2.03	0.59
3:F:12:ALA:HA	3:F:109:GLU:O	2.03	0.58
1:C:866:THR:O	1:C:870:ARG:HB2	2.02	0.58
2:K:165:ASN:O	2:K:168:SER:OG	2.21	0.58
1:C:851:LYS:HA	1:C:856:SER:HB2	1.84	0.58
1:D:696:MET:HB2	1:D:756:VAL:HG22	1.86	0.58
1:B:686:THR:O	1:B:690:SER:OG	2.22	0.58
1:D:864:ILE:O	1:D:868:PRO:HD2	2.03	0.58
1:A:484:LEU:HD23	2:E:58:SER:HB2	1.84	0.58
1:A:708:LEU:O	1:A:712:MET:HG2	2.03	0.58
2:I:60:TYR:CD1	3:J:98:ILE:HG21	2.38	0.58
3:L:40:TYR:HE2	3:L:93:GLN:HG2	1.69	0.58
2:E:60:TYR:CD1	3:F:98:ILE:HG21	2.38	0.57
1:D:413:TYR:CD1	1:D:769:LEU:HB3	2.39	0.57
1:C:411:PHE:CD1	1:C:610:VAL:HG11	2.39	0.57
3:L:189:GLU:HA	3:L:192:ARG:HG3	1.87	0.57
3:J:41:GLN:HB2	3:J:51:LEU:HD11	1.86	0.57
1:B:696:MET:HB2	1:B:756:VAL:HG22	1.85	0.57
1:D:588:LEU:HD12	1:D:609:GLY:HA2	1.87	0.57
1:B:808:ARG:NH2	1:B:840:GLN:HG3	2.19	0.57
1:A:472:GLU:OE1	1:A:490:ARG:NH1	2.38	0.57
1:B:551:LYS:O	1:B:552:THR:OG1	2.22	0.57
2:G:177:PRO:O	3:H:166:SER:OG	2.19	0.56
1:B:807:ASP:O	1:B:811:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:34:ILE:HG23	2:K:99:ARG:HD2	1.87	0.56
1:A:866:THR:O	1:A:870:ARG:HB2	2.05	0.56
2:E:6:GLU:OE2	2:E:114:GLY:HA3	2.06	0.56
2:E:6:GLU:HG3	2:E:97:CYS:HB2	1.87	0.56
3:L:197:THR:OG1	3:L:212:SER:OG	2.17	0.56
1:A:822:VAL:O	1:A:825:VAL:HG22	2.05	0.56
1:B:708:LEU:O	1:B:712:MET:HG2	2.05	0.56
2:K:11:LYS:HG3	2:K:12:LEU:N	2.20	0.56
1:A:492:TRP:CE2	1:A:664:MET:HB2	2.40	0.56
3:H:84:GLU:HA	3:H:110:ILE:CD1	2.35	0.56
1:B:658:GLU:HG2	2:G:59:LYS:HG2	1.88	0.56
1:B:864:ILE:O	1:B:868:PRO:HD2	2.06	0.56
1:A:811:LEU:HD22	1:A:826:LYS:HZ1	1.71	0.56
1:B:680:LEU:HD21	1:B:863:LEU:HD23	1.88	0.56
1:D:492:TRP:CE2	1:D:664:MET:HB2	2.41	0.56
1:D:488:VAL:HG21	1:D:654:GLY:HA2	1.87	0.56
1:A:411:PHE:CD1	1:A:610:VAL:HG11	2.40	0.55
1:B:811:LEU:HD22	1:B:826:LYS:HZ1	1.71	0.55
1:D:661:ILE:O	1:D:664:MET:HG2	2.06	0.55
1:C:865:LEU:O	1:C:869:LEU:HB3	2.06	0.55
1:B:472:GLU:OE1	1:B:490:ARG:NH1	2.40	0.55
1:D:412:ILE:HG13	1:D:734:HIS:HD2	1.70	0.55
1:C:820:PRO:HG2	1:C:822:VAL:O	2.05	0.55
1:B:845:ALA:O	1:B:849:VAL:HG23	2.06	0.55
1:B:853:THR:O	1:B:856:SER:HB3	2.07	0.55
1:D:757:LYS:HB3	1:D:759:GLN:NE2	2.21	0.55
1:C:496:TRP:CE2	1:C:668:ALA:HB2	2.41	0.55
3:F:112:ARG:HG2	3:F:113:ALA:N	2.22	0.55
1:B:402:SER:HB2	1:B:405:VAL:HG23	1.89	0.55
1:A:818:TYR:O	1:A:826:LYS:NZ	2.28	0.55
1:A:819:HIS:HA	1:A:826:LYS:HD2	1.89	0.55
1:D:734:HIS:CE1	1:D:762:SER:HG	2.25	0.55
1:B:733:THR:HG21	1:B:795:MET:HG2	1.87	0.55
1:C:490:ARG:NH2	1:C:722:PRO:HA	2.21	0.55
1:A:544:PHE:HZ	1:A:572:LEU:HD23	1.71	0.55
2:E:27:PHE:CZ	2:E:99:ARG:HD3	2.42	0.55
1:C:862:VAL:HA	1:C:865:LEU:HB3	1.87	0.55
2:I:18:LEU:HD23	2:I:84:ILE:HD12	1.89	0.55
1:B:522:GLU:OE1	1:B:805:LEU:N	2.31	0.55
1:C:853:THR:O	1:C:856:SER:HB3	2.07	0.55
1:D:807:ASP:O	1:D:811:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:ILE:HB	3:F:94:HIS:NE2	2.22	0.55
1:C:733:THR:HG21	1:C:795:MET:HG2	1.88	0.55
1:D:737:ALA:CB	1:D:738:LEU:HB2	2.33	0.54
3:J:197:THR:OG1	3:J:212:SER:OG	2.15	0.54
2:K:13:GLN:HB2	2:K:16:GLN:NE2	2.22	0.54
1:A:496:TRP:CE2	1:A:668:ALA:HB2	2.41	0.54
1:A:806:PHE:HA	1:A:809:ILE:HD12	1.88	0.54
1:C:549:LEU:HD22	1:D:569:ASN:HD21	1.72	0.54
1:D:695:LYS:HG2	1:D:755:GLU:HA	1.88	0.54
1:C:432:ARG:HG2	3:J:96:TRP:CZ3	2.42	0.54
1:D:806:PHE:HA	1:D:809:ILE:HD12	1.88	0.54
1:B:490:ARG:NH2	1:B:722:PRO:HA	2.22	0.54
2:E:34:ILE:HG23	2:E:99:ARG:HD2	1.88	0.54
1:D:658:GLU:HG2	2:K:59:LYS:HG2	1.89	0.54
1:A:658:GLU:HG2	2:E:59:LYS:HD2	1.90	0.54
1:D:432:ARG:HG2	3:L:96:TRP:CH2	2.42	0.54
2:G:54:TRP:CH2	2:G:60:TYR:HD2	2.26	0.54
1:D:829:LYS:HE2	1:D:878:PHE:CD2	2.42	0.54
1:B:651:HIS:CD2	1:B:653:LEU:HB2	2.43	0.54
1:C:829:LYS:HE2	1:C:878:PHE:CD2	2.42	0.54
2:I:29:LEU:O	2:I:55:TRP:HB2	2.06	0.54
1:A:829:LYS:HE2	1:A:878:PHE:CD2	2.43	0.54
1:A:527:LEU:HD11	1:A:848:TRP:HD1	1.73	0.54
3:F:41:GLN:HB2	3:F:51:LEU:HD11	1.90	0.54
1:A:482:ASN:HB3	2:E:56:SER:OG	2.07	0.54
3:L:84:GLU:HA	3:L:110:ILE:HD13	1.90	0.54
1:A:851:LYS:CE	1:A:859:LEU:HD22	2.34	0.54
1:B:829:LYS:HE2	1:B:878:PHE:CD2	2.42	0.54
1:C:472:GLU:OE1	1:C:490:ARG:NH1	2.40	0.54
3:F:2:ILE:HD12	3:F:94:HIS:CE1	2.42	0.54
2:I:87:VAL:HG12	2:I:121:VAL:HG11	1.89	0.54
1:B:820:PRO:HG2	1:B:822:VAL:O	2.09	0.53
1:D:845:ALA:O	1:D:849:VAL:HG23	2.09	0.53
2:I:126:THR:HG23	2:I:157:PRO:HD3	1.90	0.53
1:B:737:ALA:CB	1:B:738:LEU:HB2	2.34	0.53
1:D:657:SER:HB2	1:D:658:GLU:O	2.09	0.53
1:B:716:ALA:HB1	1:B:721:MET:HB2	1.90	0.53
1:B:851:LYS:HA	1:B:856:SER:HB2	1.91	0.53
3:J:12:ALA:HA	3:J:109:GLU:O	2.08	0.53
1:C:768:VAL:O	1:C:772:LEU:HG	2.08	0.53
1:D:866:THR:O	1:D:870:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLY:O	1:D:470:VAL:HG23	2.08	0.53
1:C:397:ILE:HG23	1:C:761:ILE:HD11	1.89	0.53
1:A:661:ILE:O	1:A:664:MET:HG2	2.09	0.53
1:D:426:LEU:O	1:D:430:LYS:HG2	2.08	0.53
3:J:40:TYR:HE2	3:J:93:GLN:CG	2.21	0.53
1:C:657:SER:HB2	1:C:658:GLU:O	2.08	0.53
1:A:651:HIS:CD2	1:A:653:LEU:H	2.27	0.53
2:G:18:LEU:HD23	2:G:84:ILE:HD12	1.90	0.53
1:D:851:LYS:HB2	1:D:859:LEU:HD13	1.91	0.53
1:B:773:SER:HA	1:B:776:MET:HG3	1.91	0.53
1:D:490:ARG:NH2	1:D:722:PRO:HA	2.23	0.53
1:C:773:SER:HA	1:C:776:MET:HG3	1.90	0.53
1:B:519:TYR:CD2	1:B:867:VAL:HG13	2.39	0.52
1:C:808:ARG:NH2	1:C:840:GLN:HG3	2.25	0.52
3:H:112:ARG:HG3	3:H:113:ALA:N	2.24	0.52
1:B:440:LEU:HD11	1:B:464:PHE:HB2	1.91	0.52
2:K:18:LEU:HD23	2:K:84:ILE:HD12	1.91	0.52
1:D:412:ILE:HG13	1:D:734:HIS:CD2	2.44	0.52
1:D:716:ALA:HB1	1:D:721:MET:HB2	1.90	0.52
1:B:520:THR:HG22	1:B:867:VAL:HG11	1.90	0.52
1:A:440:LEU:HD11	1:A:464:PHE:HB2	1.90	0.52
3:H:39:TRP:HB2	3:H:52:ILE:HB	1.92	0.52
1:A:526:PHE:HD2	1:A:844:LEU:HD21	1.74	0.52
1:C:811:LEU:HD23	1:C:814:LYS:HD2	1.91	0.52
1:B:419:PRO:O	1:B:423:PHE:HB2	2.09	0.52
1:D:853:THR:O	1:D:856:SER:HB3	2.10	0.52
1:D:773:SER:HA	1:D:776:MET:HG3	1.92	0.52
3:H:110:ILE:N	3:H:170:GLN:OE1	2.38	0.52
2:I:4:LEU:HD13	2:I:24:PHE:HB3	1.92	0.52
1:A:757:LYS:HB3	1:A:759:GLN:NE2	2.25	0.52
1:D:432:ARG:HH22	1:D:480:GLU:CD	2.14	0.52
1:C:832:ARG:HD3	1:C:835:LEU:HD12	1.92	0.52
1:B:878:PHE:HD2	1:B:882:GLU:HB3	1.74	0.51
2:K:54:TRP:CH2	2:K:60:TYR:HD2	2.28	0.51
1:C:552:THR:HB	1:C:553:TYR:HB3	1.93	0.51
1:D:836:PHE:CD2	1:D:886:LEU:HD13	2.45	0.51
1:A:597:PHE:HB3	1:A:602:ARG:HB2	1.91	0.51
1:A:426:LEU:O	1:A:430:LYS:HG2	2.10	0.51
3:J:3:VAL:HB	3:J:26:SER:HB3	1.92	0.51
1:B:811:LEU:HD23	1:B:814:LYS:HD2	1.91	0.51
1:C:551:LYS:O	1:C:552:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:40:TYR:HE2	3:F:93:GLN:HG2	1.75	0.51
3:J:52:ILE:CD1	3:J:58:LEU:HG	2.40	0.51
2:E:162:LEU:HD12	2:E:207:VAL:HG22	1.92	0.51
2:I:6:GLU:HG3	2:I:97:CYS:HB2	1.92	0.51
1:C:443:SER:OG	1:C:447:GLN:NE2	2.43	0.51
3:H:110:ILE:O	3:H:170:GLN:NE2	2.32	0.51
1:D:696:MET:HB2	1:D:756:VAL:CG2	2.41	0.51
1:A:590:LYS:O	1:A:594:SER:N	2.42	0.51
1:D:438:SER:OG	1:D:639:LYS:O	2.27	0.51
1:A:520:THR:HG22	1:A:867:VAL:CG1	2.40	0.51
1:B:526:PHE:HD2	1:B:844:LEU:HD21	1.75	0.51
1:B:803:ILE:HG22	1:B:806:PHE:H	1.74	0.51
1:D:803:ILE:HG22	1:D:806:PHE:H	1.74	0.51
1:D:811:LEU:HD22	1:D:826:LYS:NZ	2.24	0.51
1:A:657:SER:HB2	1:A:658:GLU:O	2.10	0.51
1:C:581:THR:HG21	1:C:787:VAL:HG13	1.92	0.51
1:B:739:THR:HG23	1:B:756:VAL:HG12	1.92	0.51
2:E:158:GLU:HG3	2:E:159:PRO:HA	1.92	0.51
1:C:739:THR:HG23	1:C:756:VAL:HG12	1.92	0.51
1:C:822:VAL:O	1:C:825:VAL:HG22	2.11	0.51
1:A:739:THR:HG23	1:A:756:VAL:HG12	1.92	0.51
3:L:40:TYR:HE2	3:L:93:GLN:CG	2.24	0.51
1:A:524:PHE:CZ	1:A:528:ILE:HD11	2.46	0.51
2:E:2:VAL:HG11	2:E:112:TYR:CD1	2.46	0.51
1:A:691:LYS:HD2	1:A:693:GLU:OE1	2.11	0.51
1:D:411:PHE:CD1	1:D:610:VAL:HG11	2.46	0.51
1:C:818:TYR:O	1:C:826:LYS:NZ	2.39	0.51
2:E:87:VAL:HG12	2:E:121:VAL:HG11	1.93	0.51
1:A:540:LEU:HD22	1:A:578:MET:SD	2.51	0.51
1:D:520:THR:HG22	1:D:867:VAL:HG11	1.92	0.50
1:C:864:ILE:O	1:C:868:PRO:HD2	2.10	0.50
1:B:658:GLU:HG2	2:G:59:LYS:CG	2.41	0.50
1:C:487:ILE:HG13	1:C:650:ILE:HD13	1.93	0.50
1:D:482:ASN:HB3	2:K:56:SER:OG	2.11	0.50
1:C:455:GLY:O	1:C:760:ARG:NH1	2.45	0.50
1:A:811:LEU:HD23	1:A:814:LYS:HD2	1.93	0.50
2:K:109:TYR:CZ	3:L:53:LYS:HD2	2.46	0.50
1:D:552:THR:HB	1:D:553:TYR:HB3	1.93	0.50
1:C:661:ILE:O	1:C:664:MET:HG2	2.11	0.50
1:C:651:HIS:CD2	1:C:653:LEU:HB2	2.46	0.50
1:A:689:VAL:HG12	1:A:696:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ARG:HG2	3:H:96:TRP:CZ3	2.47	0.50
1:B:696:MET:HB2	1:B:756:VAL:CG2	2.42	0.50
2:I:206:ASN:ND2	2:I:217:ASP:OD1	2.42	0.50
3:L:58:LEU:HD21	3:L:66:PHE:O	2.12	0.50
1:C:447:GLN:HE22	1:C:724:LEU:HG	1.76	0.50
1:B:661:ILE:HA	1:B:664:MET:SD	2.52	0.50
1:D:492:TRP:CD2	1:D:664:MET:HB2	2.47	0.50
1:D:472:GLU:OE1	1:D:490:ARG:NH1	2.45	0.50
1:D:820:PRO:HG2	1:D:822:VAL:O	2.12	0.50
1:C:660:PRO:HD3	2:I:58:SER:HA	1.94	0.50
1:C:737:ALA:CB	1:C:738:LEU:HB2	2.35	0.50
1:D:837:THR:O	1:D:840:GLN:HB2	2.12	0.50
1:D:808:ARG:HH22	1:D:840:GLN:HG3	1.77	0.50
1:A:584:PHE:CE2	1:A:616:ILE:HG21	2.46	0.50
1:C:426:LEU:O	1:C:430:LYS:HG2	2.12	0.50
2:I:162:LEU:HD12	2:I:207:VAL:HG22	1.94	0.49
1:B:866:THR:O	1:B:870:ARG:HB2	2.12	0.49
1:C:812:LEU:HA	1:C:834:HIS:HE1	1.77	0.49
1:C:432:ARG:HH22	1:C:480:GLU:CD	2.15	0.49
1:D:590:LYS:O	1:D:594:SER:N	2.46	0.49
1:D:519:TYR:CD2	1:D:867:VAL:HG13	2.37	0.49
1:B:492:TRP:CE2	1:B:664:MET:HB2	2.48	0.49
1:A:634:VAL:HG12	1:A:774:ILE:HD13	1.95	0.49
1:A:820:PRO:HG2	1:A:822:VAL:O	2.12	0.49
1:A:839:ILE:O	1:A:842:ILE:HG22	2.13	0.49
1:B:384:ARG:O	1:B:388:ARG:HG3	2.12	0.49
1:B:757:LYS:HB3	1:B:759:GLN:NE2	2.27	0.49
2:E:129:PRO:HB3	2:E:155:TYR:HB3	1.95	0.49
1:C:526:PHE:HD2	1:C:844:LEU:HD21	1.77	0.49
2:I:77:ASN:O	2:I:79:GLN:HG3	2.13	0.49
3:J:121:ILE:HG22	3:J:211:LYS:HE2	1.95	0.49
1:D:768:VAL:O	1:D:772:LEU:HG	2.12	0.49
2:G:34:ILE:HG23	2:G:99:ARG:HD2	1.94	0.49
3:J:117:PRO:HG3	3:J:148:ILE:HD11	1.94	0.49
1:A:397:ILE:HG23	1:A:761:ILE:HD11	1.94	0.49
1:C:651:HIS:CD2	1:C:653:LEU:H	2.31	0.49
1:D:686:THR:O	1:D:690:SER:OG	2.28	0.49
1:A:490:ARG:NH2	1:A:722:PRO:HA	2.28	0.49
1:D:658:GLU:HG2	2:K:59:LYS:CG	2.42	0.49
3:L:84:GLU:HA	3:L:110:ILE:CD1	2.43	0.48
2:K:198:TRP:CG	2:K:199:PRO:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ARG:NH2	1:A:840:GLN:HG3	2.28	0.48
1:C:757:LYS:HB3	1:C:759:GLN:NE2	2.27	0.48
1:D:496:TRP:CE2	1:D:668:ALA:HB2	2.48	0.48
1:A:389:ARG:NH2	1:A:396:ASP:OD2	2.28	0.48
1:D:811:LEU:HD13	1:D:826:LYS:HE3	1.95	0.48
1:C:487:ILE:O	1:C:491:VAL:HG23	2.13	0.48
1:A:581:THR:HG21	1:A:787:VAL:HG13	1.95	0.48
1:B:382:LEU:HB2	1:B:703:HIS:HB3	1.95	0.48
1:B:413:TYR:CE1	1:B:769:LEU:HB3	2.49	0.48
1:C:811:LEU:HD22	1:C:826:LYS:HZ1	1.78	0.48
1:A:657:SER:HB2	1:A:658:GLU:C	2.34	0.48
1:A:864:ILE:O	1:A:868:PRO:HD2	2.14	0.48
1:B:837:THR:O	1:B:840:GLN:HB2	2.13	0.48
1:D:780:LEU:HA	1:D:783:ILE:HD12	1.94	0.48
1:A:466:GLY:O	1:A:470:VAL:HG23	2.14	0.48
2:E:181:GLN:O	2:E:181:GLN:HG3	2.14	0.48
1:A:853:THR:O	1:A:856:SER:HB3	2.13	0.48
1:D:811:LEU:HD23	1:D:814:LYS:HD2	1.94	0.48
1:C:786:ALA:O	1:C:789:PHE:HB2	2.14	0.48
2:E:137:VAL:HG22	3:F:123:PRO:HD3	1.95	0.48
1:D:453:LEU:O	1:D:760:ARG:NH1	2.47	0.48
1:D:447:GLN:HE21	1:D:712:MET:HB2	1.78	0.48
2:I:54:TRP:CH2	2:I:60:TYR:HD2	2.31	0.48
1:C:590:LYS:O	1:C:594:SER:N	2.47	0.48
1:D:865:LEU:O	1:D:869:LEU:HB3	2.14	0.48
2:K:89:THR:HA	2:K:121:VAL:HB	1.95	0.48
1:A:520:THR:CG2	1:A:867:VAL:HG11	2.44	0.48
3:L:110:ILE:O	3:L:170:GLN:NE2	2.43	0.48
3:F:11:LEU:HG	3:F:13:VAL:HG23	1.95	0.48
1:A:865:LEU:O	1:A:869:LEU:HB3	2.13	0.48
2:I:37:GLY:HA3	2:I:52:HIS:CG	2.49	0.48
1:B:411:PHE:CD1	1:B:610:VAL:HG11	2.48	0.48
1:A:527:LEU:CD1	1:A:848:TRP:HD1	2.27	0.48
1:D:862:VAL:HA	1:D:865:LEU:HB3	1.95	0.48
3:J:214:ASN:HB2	3:J:217:GLU:HB3	1.96	0.48
1:A:737:ALA:CB	1:A:738:LEU:HB2	2.34	0.47
1:A:836:PHE:CD2	1:A:886:LEU:HD13	2.49	0.47
1:A:569:ASN:HD21	1:B:549:LEU:HD22	1.79	0.47
3:F:30:SER:HB3	3:F:35:SER:HA	1.95	0.47
1:C:440:LEU:HD11	1:C:464:PHE:HB2	1.95	0.47
1:A:847:LEU:HD21	1:A:863:LEU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:HIS:HA	1:C:826:LYS:HD2	1.97	0.47
1:A:757:LYS:HB3	1:A:759:GLN:HE22	1.79	0.47
1:B:634:VAL:HG12	1:B:774:ILE:HD13	1.96	0.47
2:G:109:TYR:CZ	3:H:53:LYS:HD2	2.50	0.47
2:K:129:PRO:HB3	2:K:155:TYR:HB3	1.95	0.47
1:D:808:ARG:HH21	1:D:837:THR:HA	1.79	0.47
1:A:544:PHE:CZ	1:A:572:LEU:HD23	2.49	0.47
2:E:109:TYR:CZ	3:F:53:LYS:HD2	2.50	0.47
1:C:520:THR:HG22	1:C:867:VAL:CG1	2.44	0.47
1:B:657:SER:HB2	1:B:658:GLU:O	2.14	0.47
1:D:878:PHE:HD2	1:D:882:GLU:HB3	1.79	0.47
4:B:1000:4KU:H7	4:B:1000:4KU:H11	1.43	0.47
3:J:112:ARG:HG2	3:J:113:ALA:N	2.30	0.47
1:A:519:TYR:CD2	1:A:867:VAL:HG13	2.47	0.47
1:D:390:TYR:O	1:D:393:TYR:HB3	2.15	0.47
1:B:657:SER:HB2	1:B:658:GLU:C	2.35	0.47
1:C:777:GLU:HB3	1:C:778:PRO:HD3	1.96	0.47
1:B:479:CYS:HA	1:B:484:LEU:HD12	1.97	0.47
1:D:733:THR:HG21	1:D:795:MET:HG2	1.97	0.47
1:B:404:GLN:HG2	1:B:738:LEU:H	1.80	0.47
1:C:519:TYR:CD2	1:C:867:VAL:HG13	2.47	0.47
2:I:92:THR:HG23	2:I:120:THR:HA	1.97	0.47
3:F:116:ALA:HA	3:F:204:THR:HG21	1.97	0.47
2:K:153:LYS:HG2	2:K:154:GLY:N	2.30	0.47
1:A:588:LEU:HD12	1:A:609:GLY:HA2	1.96	0.47
1:B:865:LEU:O	1:B:869:LEU:HB3	2.15	0.47
3:J:39:TRP:CZ3	3:J:92:CYS:HB3	2.49	0.47
2:K:41:GLN:HG3	2:K:46:GLY:O	2.15	0.47
1:C:597:PHE:HB3	1:C:602:ARG:HB2	1.95	0.47
3:F:189:GLU:HA	3:F:192:ARG:HG3	1.97	0.46
1:B:812:LEU:HA	1:B:834:HIS:CE1	2.50	0.46
1:A:443:SER:O	1:A:447:GLN:HB2	2.16	0.46
1:B:780:LEU:HA	1:B:783:ILE:HD12	1.97	0.46
1:C:630:GLN:HB3	1:C:785:LEU:HD12	1.97	0.46
1:A:678:ILE:HG12	1:A:725:SER:HB3	1.95	0.46
3:J:112:ARG:NH1	3:J:174:ASP:HB2	2.26	0.46
1:C:432:ARG:O	1:C:433:ASN:HB2	2.15	0.46
1:C:402:SER:HB2	1:C:405:VAL:HG23	1.98	0.46
3:H:40:TYR:HE2	3:H:93:GLN:HG2	1.80	0.46
1:C:485:GLU:OE2	1:C:655:LEU:HB2	2.14	0.46
2:I:131:VAL:HB	2:I:216:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:SER:HA	1:B:541:ILE:HG22	1.98	0.46
1:D:715:VAL:O	1:D:719:PHE:HD1	1.97	0.46
1:A:863:LEU:O	1:A:867:VAL:HG23	2.16	0.46
2:G:179:VAL:HG21	3:H:165:ASN:O	2.15	0.46
2:E:77:ASN:O	2:E:79:GLN:HG3	2.16	0.46
2:I:5:GLN:O	2:I:22:CYS:HA	2.14	0.46
1:D:547:HIS:ND1	1:D:567:LEU:HA	2.30	0.46
1:C:839:ILE:O	1:C:842:ILE:HG22	2.16	0.46
1:C:878:PHE:HD2	1:C:882:GLU:HB3	1.80	0.46
2:G:11:LYS:HB2	2:G:157:PRO:HG3	1.97	0.46
3:J:29:VAL:HG21	3:J:94:HIS:HB2	1.96	0.46
1:B:808:ARG:HH22	1:B:840:GLN:HG3	1.80	0.46
1:D:513:VAL:HG11	1:D:702:PHE:CE2	2.50	0.46
3:H:164:LEU:O	3:H:164:LEU:HD12	2.16	0.46
1:D:487:ILE:HG13	1:D:650:ILE:HD13	1.98	0.46
1:A:768:VAL:O	1:A:772:LEU:HG	2.16	0.46
2:G:102:TYR:CZ	2:G:106:GLY:HA2	2.51	0.46
2:K:53:ILE:HD12	2:K:59:LYS:HE2	1.98	0.46
1:B:862:VAL:HA	1:B:865:LEU:HB3	1.97	0.46
1:D:777:GLU:HB3	1:D:778:PRO:HD3	1.97	0.46
1:D:584:PHE:CE2	1:D:616:ILE:HG21	2.51	0.46
2:K:101:TYR:O	2:K:108:TYR:HA	2.16	0.45
1:B:872:VAL:O	1:B:875:PRO:HD2	2.15	0.45
1:A:851:LYS:HA	1:A:856:SER:HB2	1.98	0.45
1:A:812:LEU:HA	1:A:834:HIS:HE1	1.78	0.45
1:C:414:PHE:CE1	1:C:783:ILE:HD13	2.51	0.45
1:B:513:VAL:HG11	1:B:702:PHE:CE2	2.51	0.45
3:L:51:LEU:HA	3:L:62:VAL:HG21	1.98	0.45
3:J:7:SER:HB2	3:J:8:PRO:HA	1.97	0.45
1:C:738:LEU:O	1:C:756:VAL:HB	2.15	0.45
1:A:738:LEU:O	1:A:756:VAL:HB	2.16	0.45
1:B:808:ARG:HH21	1:B:837:THR:HA	1.80	0.45
1:B:835:LEU:O	1:B:839:ILE:HG13	2.17	0.45
3:L:93:GLN:HB3	3:L:102:PHE:CD2	2.51	0.45
1:A:440:LEU:HA	1:A:722:PRO:HG3	1.97	0.45
1:B:768:VAL:O	1:B:772:LEU:HG	2.16	0.45
1:D:419:PRO:O	1:D:423:PHE:HB2	2.15	0.45
1:A:873:LEU:O	1:A:876:LEU:HB3	2.17	0.45
2:E:4:LEU:HD13	2:E:24:PHE:HB3	1.98	0.45
1:C:657:SER:HB2	1:C:658:GLU:C	2.37	0.45
1:D:526:PHE:HD2	1:D:844:LEU:HD21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:LYS:HB3	1:B:759:GLN:HE22	1.80	0.45
2:G:129:PRO:HB3	2:G:155:TYR:HB3	1.98	0.45
1:A:845:ALA:O	1:A:849:VAL:HG23	2.17	0.45
2:I:3:LYS:HD3	2:I:3:LYS:HA	1.79	0.45
3:J:129:LEU:O	3:J:187:LYS:HD2	2.16	0.45
1:A:651:HIS:HA	1:A:652:PRO:HD2	1.82	0.45
1:A:412:ILE:HA	1:A:415:ALA:HB3	1.97	0.45
1:B:438:SER:OG	1:B:639:LYS:O	2.33	0.45
3:J:51:LEU:HA	3:J:62:VAL:HG21	1.99	0.45
1:A:596:TYR:O	1:A:602:ARG:HD2	2.17	0.45
1:D:384:ARG:O	1:D:388:ARG:HG3	2.15	0.45
1:A:439:GLU:OE2	1:A:640:VAL:HG13	2.17	0.45
1:B:485:GLU:OE2	1:B:655:LEU:HB2	2.17	0.45
3:L:164:LEU:HD12	3:L:164:LEU:O	2.17	0.45
1:C:849:VAL:O	1:C:852:SER:HB3	2.17	0.45
3:J:2:ILE:HD12	3:J:94:HIS:CE1	2.52	0.45
1:D:657:SER:HB2	1:D:658:GLU:C	2.37	0.45
1:B:715:VAL:O	1:B:719:PHE:HD1	2.00	0.45
1:C:439:GLU:OE2	1:C:640:VAL:HG13	2.17	0.45
4:D:1000:4KU:H7	4:D:1000:4KU:H11	1.45	0.45
1:B:432:ARG:HH22	1:B:480:GLU:CD	2.20	0.45
1:B:822:VAL:O	1:B:825:VAL:HG22	2.16	0.45
2:I:69:LEU:CD2	2:I:84:ILE:HG12	2.47	0.45
1:D:468:LEU:O	1:D:472:GLU:HG2	2.17	0.45
1:A:849:VAL:O	1:A:852:SER:HB3	2.17	0.45
1:C:845:ALA:O	1:C:849:VAL:HG23	2.16	0.45
1:D:842:ILE:O	1:D:846:VAL:HG23	2.17	0.45
1:C:629:THR:HB	1:C:631:LYS:HE2	1.99	0.45
1:C:695:LYS:HB3	1:C:755:GLU:HA	1.98	0.45
1:B:839:ILE:O	1:B:842:ILE:HG22	2.17	0.45
1:C:870:ARG:O	1:C:874:LEU:N	2.50	0.45
2:I:162:LEU:HA	2:I:206:ASN:O	2.16	0.45
1:A:733:THR:HG21	1:A:795:MET:HG2	1.99	0.45
1:B:482:ASN:HB3	2:G:56:SER:OG	2.17	0.45
1:B:877:ILE:HA	1:B:877:ILE:HD13	1.81	0.45
1:A:878:PHE:HD2	1:A:882:GLU:HB3	1.82	0.44
1:C:696:MET:HB2	1:C:756:VAL:HG22	1.97	0.44
1:D:487:ILE:O	1:D:491:VAL:HG23	2.16	0.44
2:I:38:TRP:CD1	2:I:82:LEU:HB2	2.52	0.44
3:L:39:TRP:HB2	3:L:52:ILE:HB	1.99	0.44
1:D:765:LEU:O	1:D:769:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:191:GLU:HA	3:J:215:ARG:CD	2.47	0.44
3:J:119:VAL:HA	3:J:139:PHE:O	2.18	0.44
1:A:658:GLU:HG2	2:E:59:LYS:CG	2.47	0.44
1:A:808:ARG:HH21	1:A:837:THR:HA	1.83	0.44
3:H:116:ALA:HA	3:H:204:THR:HG21	1.98	0.44
1:A:389:ARG:HD2	1:A:389:ARG:HA	1.74	0.44
1:D:494:GLY:O	1:D:498:ILE:HG13	2.16	0.44
1:C:524:PHE:CZ	1:C:528:ILE:HD11	2.52	0.44
1:B:727:THR:HG21	1:B:730:ARG:NH2	2.32	0.44
1:A:551:LYS:HE2	1:A:551:LYS:HB3	1.65	0.44
1:B:583:PHE:HD2	1:B:584:PHE:HD1	1.64	0.44
1:D:404:GLN:HG2	1:D:738:LEU:H	1.82	0.44
2:G:29:LEU:O	2:G:55:TRP:HB2	2.18	0.44
1:D:443:SER:HB2	1:D:721:MET:HB3	1.99	0.44
1:A:780:LEU:HA	1:A:783:ILE:HD12	2.00	0.44
1:D:651:HIS:CD2	1:D:653:LEU:HB2	2.52	0.44
1:A:382:LEU:HA	1:A:703:HIS:ND1	2.32	0.44
2:E:69:LEU:HD22	2:E:82:LEU:HD11	2.00	0.44
1:A:777:GLU:HB3	1:A:778:PRO:HD3	1.98	0.44
3:F:121:ILE:HG22	3:F:211:LYS:HE2	2.00	0.44
1:A:455:GLY:O	1:A:760:ARG:NH1	2.50	0.44
1:B:458:PRO:HB3	1:B:760:ARG:HD3	2.00	0.44
2:K:11:LYS:HB3	2:K:157:PRO:HG3	1.98	0.44
2:K:109:TYR:HB3	3:L:38:ASN:ND2	2.32	0.44
2:K:153:LYS:HG2	2:K:154:GLY:H	1.82	0.44
2:G:41:GLN:HG3	2:G:46:GLY:O	2.17	0.44
1:B:853:THR:HB	1:B:855:ALA:HB3	2.00	0.44
1:B:849:VAL:O	1:B:852:SER:HB3	2.18	0.44
2:K:13:GLN:HB2	2:K:16:GLN:CD	2.38	0.44
1:C:551:LYS:HB3	1:C:551:LYS:HE2	1.67	0.44
1:B:777:GLU:HB3	1:B:778:PRO:HD3	1.99	0.44
1:B:695:LYS:HG2	1:B:755:GLU:HA	2.00	0.44
1:D:634:VAL:HG12	1:D:774:ILE:HD13	1.99	0.44
1:D:691:LYS:HE2	1:D:694:ARG:HE	1.82	0.44
1:C:740:VAL:HB	1:C:754:GLN:HB3	2.00	0.44
1:D:822:VAL:O	1:D:825:VAL:HG22	2.17	0.44
2:K:105:TYR:HB2	3:L:54:TYR:CE1	2.53	0.44
2:G:198:TRP:CG	2:G:199:PRO:HA	2.52	0.44
1:C:877:ILE:HA	1:C:877:ILE:HD13	1.82	0.44
1:C:678:ILE:HG12	1:C:725:SER:HB3	1.99	0.44
1:A:818:TYR:C	1:A:826:LYS:HZ3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:LYS:O	1:D:552:THR:OG1	2.26	0.44
1:A:414:PHE:CE1	1:A:783:ILE:HD13	2.52	0.44
2:I:41:GLN:HG3	2:I:46:GLY:O	2.17	0.44
3:F:165:ASN:HA	3:F:180:SER:O	2.18	0.44
3:F:190:TYR:CZ	3:F:215:ARG:HG3	2.53	0.44
1:D:389:ARG:HG3	1:D:760:ARG:NH2	2.33	0.43
1:D:839:ILE:O	1:D:842:ILE:HG22	2.18	0.43
3:J:116:ALA:HA	3:J:204:THR:HG21	2.00	0.43
3:J:29:VAL:CG2	3:J:96:TRP:HB2	2.45	0.43
1:B:447:GLN:HE21	1:B:712:MET:HB2	1.83	0.43
1:B:552:THR:HB	1:B:553:TYR:HB3	1.99	0.43
2:G:153:LYS:HG2	2:G:154:GLY:N	2.33	0.43
1:A:686:THR:O	1:A:690:SER:OG	2.33	0.43
3:J:13:VAL:CG1	3:J:17:GLN:HB3	2.48	0.43
1:B:487:ILE:O	1:B:491:VAL:HG23	2.17	0.43
1:A:660:PRO:HD3	2:E:58:SER:HA	1.99	0.43
1:A:581:THR:OG1	1:A:617:MET:HG3	2.18	0.43
1:C:416:ALA:HA	1:C:730:ARG:HD3	2.00	0.43
1:D:551:LYS:HE2	1:D:551:LYS:HB3	1.64	0.43
1:A:487:ILE:O	1:A:491:VAL:HG23	2.18	0.43
1:D:443:SER:O	1:D:447:GLN:HB2	2.19	0.43
1:C:658:GLU:HG2	2:I:59:LYS:HD2	2.00	0.43
1:A:820:PRO:HD3	1:A:826:LYS:CD	2.46	0.43
2:E:34:ILE:CG2	2:E:99:ARG:HD2	2.49	0.43
2:E:158:GLU:HG3	2:E:159:PRO:CA	2.49	0.43
2:E:109:TYR:HB3	3:F:38:ASN:ND2	2.33	0.43
1:B:510:SER:O	1:B:513:VAL:HB	2.18	0.43
3:F:129:LEU:O	3:F:187:LYS:HD2	2.19	0.43
2:K:181:GLN:O	2:K:181:GLN:HG3	2.19	0.43
2:K:29:LEU:O	2:K:55:TRP:HB2	2.19	0.43
2:G:18:LEU:HD13	2:G:119:LEU:HD13	2.01	0.43
1:A:429:GLU:OE2	3:F:32:SER:HB3	2.18	0.43
2:I:137:VAL:HG22	3:J:123:PRO:HD3	2.00	0.43
1:A:547:HIS:ND1	1:A:567:LEU:HA	2.34	0.43
1:C:753:ILE:HD12	1:C:753:ILE:N	2.33	0.43
1:B:389:ARG:HG3	1:B:760:ARG:NH2	2.34	0.43
3:H:153:LYS:HB2	3:H:197:THR:HB	2.01	0.43
3:F:40:TYR:HE2	3:F:93:GLN:CG	2.31	0.43
1:A:715:VAL:O	1:A:718:LEU:HB3	2.19	0.43
2:G:89:THR:HA	2:G:121:VAL:HB	2.00	0.43
1:A:853:THR:HB	1:A:855:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:851:LYS:HB2	1:B:859:LEU:HD13	2.01	0.43
1:C:806:PHE:HA	1:C:809:ILE:HD12	2.00	0.43
1:D:413:TYR:CE1	1:D:769:LEU:HB3	2.54	0.43
1:A:837:THR:O	1:A:840:GLN:HB2	2.19	0.43
2:G:153:LYS:HG2	2:G:154:GLY:H	1.84	0.43
1:D:740:VAL:HB	1:D:754:GLN:HB3	2.01	0.43
3:H:117:PRO:HG3	3:H:148:ILE:HD11	2.01	0.43
1:B:429:GLU:OE1	3:H:31:THR:HB	2.19	0.43
2:I:198:TRP:CG	2:I:199:PRO:HA	2.53	0.42
1:A:484:LEU:HD13	1:A:663:MET:HG2	2.01	0.42
3:L:40:TYR:CE2	3:L:93:GLN:HG2	2.51	0.42
3:F:191:GLU:HA	3:F:215:ARG:CD	2.49	0.42
2:E:198:TRP:CG	2:E:199:PRO:HA	2.53	0.42
1:B:496:TRP:CE2	1:B:668:ALA:HB2	2.54	0.42
3:F:20:THR:HG22	3:F:78:ASN:OD1	2.18	0.42
1:A:812:LEU:HD22	1:A:834:HIS:ND1	2.34	0.42
1:D:526:PHE:CE1	1:D:800:LEU:HD11	2.54	0.42
1:B:487:ILE:HD11	1:B:720:GLY:HA2	2.00	0.42
3:L:112:ARG:HG3	3:L:113:ALA:N	2.34	0.42
2:I:60:TYR:CD2	3:J:98:ILE:HG12	2.53	0.42
2:I:209:HIS:CE1	2:I:211:ALA:HB3	2.53	0.42
2:I:6:GLU:OE2	2:I:114:GLY:HA3	2.19	0.42
1:B:754:GLN:HG3	1:B:755:GLU:OE1	2.19	0.42
3:F:62:VAL:HA	3:F:63:PRO:HD3	1.84	0.42
1:A:432:ARG:HG2	3:F:96:TRP:CZ3	2.54	0.42
1:A:482:ASN:HB3	2:E:56:SER:HG	1.82	0.42
1:C:405:VAL:HG22	1:C:759:GLN:NE2	2.34	0.42
2:G:109:TYR:HB3	3:H:38:ASN:ND2	2.34	0.42
2:E:22:CYS:HB2	2:E:38:TRP:CZ2	2.55	0.42
1:D:651:HIS:NE2	1:D:653:LEU:HB2	2.35	0.42
3:F:43:LYS:HE2	3:F:85:GLU:O	2.18	0.42
1:D:597:PHE:HB3	1:D:602:ARG:HB2	2.01	0.42
1:D:440:LEU:HD11	1:D:464:PHE:HB2	2.00	0.42
1:A:678:ILE:HG21	1:A:710:VAL:HG22	2.01	0.42
1:C:660:PRO:HG3	2:I:58:SER:HB2	2.02	0.42
1:B:812:LEU:HD22	1:B:834:HIS:ND1	2.35	0.42
2:I:13:GLN:HB2	2:I:16:GLN:CD	2.40	0.42
2:I:113:TRP:CE3	3:J:48:PRO:HD2	2.55	0.42
2:K:18:LEU:HD13	2:K:119:LEU:HD13	2.01	0.42
1:A:862:VAL:HA	1:A:865:LEU:HB3	2.01	0.42
1:A:487:ILE:HD11	1:A:720:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:37:GLY:HA3	2:K:52:HIS:CG	2.55	0.42
1:B:622:PHE:HD1	1:B:623:PHE:CD1	2.38	0.42
1:B:494:GLY:O	1:B:498:ILE:HG13	2.19	0.42
1:B:432:ARG:HG2	3:H:96:TRP:CH2	2.54	0.42
3:H:52:ILE:HD13	3:H:58:LEU:HA	2.02	0.42
1:A:458:PRO:HB3	1:A:760:ARG:HD3	2.02	0.42
1:C:510:SER:O	1:C:513:VAL:HB	2.20	0.42
1:D:629:THR:HB	1:D:631:LYS:HE2	2.01	0.42
3:J:40:TYR:CE2	3:J:93:GLN:HG2	2.50	0.42
1:C:820:PRO:HD3	1:C:826:LYS:CD	2.48	0.42
3:F:93:GLN:HE21	3:F:93:GLN:HB2	1.61	0.42
1:C:510:SER:HG	1:C:703:HIS:HE2	1.67	0.42
1:A:665:PHE:HA	1:A:665:PHE:HD1	1.71	0.42
1:C:678:ILE:HG21	1:C:710:VAL:HG22	2.00	0.42
1:D:389:ARG:HD2	1:D:389:ARG:HA	1.72	0.42
1:C:432:ARG:HG2	3:J:96:TRP:CH2	2.55	0.42
1:B:804:GLN:HG2	1:B:808:ARG:HH11	1.85	0.42
2:I:221:GLU:HA	2:I:222:PRO:HD3	1.92	0.42
1:A:616:ILE:O	1:A:620:VAL:HG23	2.20	0.42
2:I:157:PRO:HD2	2:I:211:ALA:CB	2.50	0.42
1:D:870:ARG:O	1:D:874:LEU:N	2.53	0.42
3:F:93:GLN:HB3	3:F:102:PHE:CD2	2.55	0.42
1:A:485:GLU:OE2	1:A:655:LEU:HB2	2.19	0.42
3:L:214:ASN:HB2	3:L:217:GLU:HB3	2.02	0.42
1:B:870:ARG:O	1:B:874:LEU:N	2.53	0.41
1:A:382:LEU:HB2	1:A:703:HIS:HB3	2.02	0.41
1:B:382:LEU:HA	1:B:703:HIS:ND1	2.35	0.41
1:C:510:SER:HG	1:C:703:HIS:CD2	2.37	0.41
1:C:466:GLY:O	1:C:470:VAL:HG23	2.20	0.41
1:C:836:PHE:CD2	1:C:886:LEU:HD13	2.55	0.41
3:L:24:ARG:HA	3:L:73:THR:O	2.20	0.41
2:I:181:GLN:HG3	2:I:181:GLN:O	2.20	0.41
2:G:126:THR:HG22	2:G:157:PRO:HD3	2.02	0.41
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.86	0.41
1:C:520:THR:CG2	1:C:867:VAL:HG11	2.49	0.41
2:I:153:LYS:NZ	3:J:184:THR:HG21	2.35	0.41
1:D:851:LYS:HE2	4:D:1000:4KU:H2	1.73	0.41
1:B:678:ILE:HG21	1:B:710:VAL:HG22	2.02	0.41
1:C:810:LEU:HB3	1:C:814:LYS:HE2	2.01	0.41
1:B:492:TRP:CD2	1:B:664:MET:HB2	2.55	0.41
1:D:584:PHE:HE2	1:D:616:ILE:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:116:ALA:HA	3:L:204:THR:HG21	2.02	0.41
1:B:851:LYS:HE2	4:B:1000:4KU:H2	1.77	0.41
1:A:413:TYR:CE1	1:A:769:LEU:HB3	2.56	0.41
1:A:653:LEU:HD13	1:A:653:LEU:HA	1.66	0.41
3:H:93:GLN:HB3	3:H:102:PHE:CD2	2.56	0.41
3:H:40:TYR:HE2	3:H:93:GLN:CG	2.33	0.41
1:B:487:ILE:HG13	1:B:650:ILE:HD13	2.03	0.41
1:B:524:PHE:CZ	1:B:528:ILE:HD11	2.55	0.41
1:B:526:PHE:CE1	1:B:800:LEU:HD11	2.55	0.41
1:D:583:PHE:HD2	1:D:584:PHE:HD1	1.67	0.41
2:I:105:TYR:HD2	3:J:54:TYR:CE2	2.39	0.41
1:C:457:GLN:HG3	1:C:460:LEU:HG	2.02	0.41
2:I:109:TYR:CZ	3:J:53:LYS:HD2	2.56	0.41
1:D:393:TYR:HD1	1:D:760:ARG:NE	2.18	0.41
1:B:820:PRO:HD3	1:B:826:LYS:CD	2.49	0.41
1:B:765:LEU:O	1:B:769:LEU:HB2	2.21	0.41
1:A:870:ARG:O	1:A:874:LEU:N	2.53	0.41
1:C:808:ARG:HH21	1:C:837:THR:HA	1.86	0.41
1:C:583:PHE:HD2	1:C:584:PHE:HD1	1.68	0.41
1:B:390:TYR:O	1:B:393:TYR:HB3	2.21	0.41
2:E:105:TYR:HB2	3:F:54:TYR:CE1	2.56	0.41
1:D:439:GLU:OE2	1:D:640:VAL:HG13	2.19	0.41
1:D:518:ARG:HB3	1:D:887:ASP:HB2	2.03	0.41
1:D:432:ARG:NH2	1:D:480:GLU:OE1	2.53	0.41
1:D:661:ILE:HA	1:D:664:MET:SD	2.61	0.41
1:D:849:VAL:O	1:D:852:SER:HB3	2.21	0.41
3:J:16:GLY:HA2	3:J:81:PRO:HB2	2.03	0.41
1:D:812:LEU:HD22	1:D:834:HIS:ND1	2.36	0.41
1:C:715:VAL:O	1:C:718:LEU:HB3	2.21	0.41
2:K:22:CYS:HB2	2:K:38:TRP:CZ2	2.56	0.41
1:B:389:ARG:HA	1:B:389:ARG:HD2	1.73	0.41
1:C:807:ASP:O	1:C:811:LEU:HG	2.20	0.41
4:C:1000:4KU:SAG	4:C:1000:4KU:H6	2.61	0.41
1:A:583:PHE:HD2	1:A:584:PHE:HD1	1.68	0.41
1:D:494:GLY:O	1:D:497:LEU:HB2	2.21	0.41
1:B:691:LYS:HE2	1:B:694:ARG:HE	1.86	0.41
1:B:463:GLY:HA2	1:B:724:LEU:HD13	2.02	0.41
1:D:524:PHE:CZ	1:D:528:ILE:HD11	2.56	0.41
4:C:1000:4KU:H7	4:C:1000:4KU:H11	1.49	0.40
3:F:40:TYR:CE2	3:F:93:GLN:HG2	2.56	0.40
2:K:77:ASN:O	2:K:79:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:PHE:HD2	1:A:676:ILE:HD13	1.85	0.40
2:E:18:LEU:HD23	2:E:84:ILE:HD12	2.03	0.40
1:D:808:ARG:HH22	1:D:840:GLN:NE2	2.19	0.40
1:C:811:LEU:HD22	1:C:826:LYS:NZ	2.37	0.40
1:C:393:TYR:HD1	1:C:760:ARG:NE	2.19	0.40
1:A:635:PRO:HG2	1:A:774:ILE:HD11	2.03	0.40
1:B:740:VAL:HB	1:B:754:GLN:HB3	2.03	0.40
2:K:122:SER:HG	2:K:156:PHE:HE1	1.67	0.40
1:A:683:GLN:OE1	1:A:702:PHE:HD2	2.05	0.40
1:A:695:LYS:HB3	1:A:755:GLU:HA	2.03	0.40
1:D:815:PRO:HG2	1:D:818:TYR:HD2	1.86	0.40
1:C:527:LEU:HD11	1:C:848:TRP:HD1	1.86	0.40
1:A:696:MET:HB2	1:A:756:VAL:HG22	2.02	0.40
1:D:393:TYR:HD1	1:D:760:ARG:CZ	2.34	0.40
1:C:468:LEU:O	1:C:472:GLU:HG2	2.20	0.40
2:E:3:LYS:HB2	2:E:25:SER:OG	2.22	0.40
1:D:539:LYS:O	1:D:542:LYS:HB3	2.22	0.40
2:E:29:LEU:O	2:E:55:TRP:HB2	2.22	0.40
1:A:447:GLN:HE21	1:A:712:MET:HB2	1.87	0.40
1:A:484:LEU:HD21	2:E:56:SER:HB3	2.03	0.40
1:B:651:HIS:HA	1:B:652:PRO:HD2	1.94	0.40
1:D:874:LEU:HA	1:D:874:LEU:HD23	1.92	0.40
2:G:99:ARG:HG3	2:G:100:ALA:N	2.36	0.40
2:E:221:GLU:HA	2:E:222:PRO:HD3	1.86	0.40
1:C:634:VAL:HG12	1:C:774:ILE:HD13	2.03	0.40
1:D:628:TYR:OH	1:D:630:GLN:HG2	2.21	0.40
1:B:734:HIS:CE1	1:B:762:SER:HG	2.38	0.40
3:H:121:ILE:HG22	3:H:211:LYS:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	467/911 (51%)	435 (93%)	31 (7%)	1 (0%)	52 88
1	B	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	52 88
1	C	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	52 88
1	D	467/911 (51%)	436 (93%)	30 (6%)	1 (0%)	52 88
2	E	221/223 (99%)	211 (96%)	7 (3%)	3 (1%)	14 58
2	G	221/223 (99%)	214 (97%)	7 (3%)	0	100 100
2	I	221/223 (99%)	212 (96%)	6 (3%)	3 (1%)	14 58
2	K	221/223 (99%)	213 (96%)	8 (4%)	0	100 100
3	F	216/218 (99%)	208 (96%)	8 (4%)	0	100 100
3	H	216/218 (99%)	209 (97%)	7 (3%)	0	100 100
3	J	216/218 (99%)	209 (97%)	7 (3%)	0	100 100
3	L	216/218 (99%)	211 (98%)	5 (2%)	0	100 100
All	All	3616/5408 (67%)	3430 (95%)	176 (5%)	10 (0%)	46 84

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	166	SER
2	I	166	SER
2	E	159	PRO
2	I	159	PRO
2	E	210	PRO
2	I	210	PRO
1	B	598	PRO
1	C	598	PRO
1	A	598	PRO
1	D	598	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/786 (53%)	411 (99%)	6 (1%)	74	91
1	B	417/786 (53%)	413 (99%)	4 (1%)	82	93
1	C	417/786 (53%)	412 (99%)	5 (1%)	78	92
1	D	417/786 (53%)	413 (99%)	4 (1%)	82	93
2	E	190/190 (100%)	188 (99%)	2 (1%)	80	92
2	G	190/190 (100%)	188 (99%)	2 (1%)	80	92
2	I	190/190 (100%)	187 (98%)	3 (2%)	70	89
2	K	190/190 (100%)	189 (100%)	1 (0%)	92	97
3	F	193/193 (100%)	191 (99%)	2 (1%)	82	93
3	H	193/193 (100%)	191 (99%)	2 (1%)	82	93
3	J	193/193 (100%)	191 (99%)	2 (1%)	82	93
3	L	193/193 (100%)	190 (98%)	3 (2%)	70	89
All	All	3200/4676 (68%)	3164 (99%)	36 (1%)	80	92

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	LEU
1	A	544	PHE
1	A	581	THR
1	A	588	LEU
1	A	597	PHE
1	A	723	TRP
1	B	382	LEU
1	B	544	PHE
1	B	597	PHE
1	B	607	ASP
1	C	382	LEU
1	C	544	PHE
1	C	597	PHE
1	C	607	ASP
1	C	723	TRP
1	D	382	LEU
1	D	544	PHE
1	D	597	PHE
1	D	723	TRP

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Mol	Chain	Res	Type
2	E	63	THR
2	E	222	PRO
3	F	93	GLN
3	F	168	THR
2	G	63	THR
2	G	126	THR
3	H	93	GLN
3	H	168	THR
2	I	54	TRP
2	I	199	PRO
2	I	222	PRO
3	J	93	GLN
3	J	168	THR
2	K	63	THR
3	L	58	LEU
3	L	93	GLN
3	L	168	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	GLN
1	A	651	HIS
1	A	834	HIS
1	B	569	ASN
1	C	447	GLN
1	C	651	HIS
1	C	834	HIS
1	D	840	GLN
3	H	80	HIS
3	L	80	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	4KU	A	1000	1	29,29,29	1.65	2 (6%)	32,42,42	3.68	12 (37%)
4	4KU	B	1000	1	29,29,29	1.63	4 (13%)	32,42,42	3.18	12 (37%)
4	4KU	C	1000	1	29,29,29	1.64	2 (6%)	32,42,42	3.00	10 (31%)
4	4KU	D	1000	1	29,29,29	1.67	3 (10%)	32,42,42	2.96	10 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4KU	A	1000	1	-	0/21/23/23	0/2/2/2
4	4KU	B	1000	1	-	0/21/23/23	0/2/2/2
4	4KU	C	1000	1	-	0/21/23/23	0/2/2/2
4	4KU	D	1000	1	-	0/21/23/23	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	4KU	CAI-SAG	-5.95	1.66	1.81
4	D	1000	4KU	CAI-SAG	-5.79	1.66	1.81
4	C	1000	4KU	CAI-SAG	-5.68	1.66	1.81
4	B	1000	4KU	CAI-SAG	-5.60	1.67	1.81
4	D	1000	4KU	CAJ-SAH	-5.59	1.67	1.81
4	B	1000	4KU	CAJ-SAH	-5.46	1.67	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1000	4KU	CAJ-SAH	-5.45	1.67	1.81
4	A	1000	4KU	CAJ-SAH	-5.26	1.67	1.81
4	B	1000	4KU	CAU-NAS	2.01	1.44	1.38
4	B	1000	4KU	CAV-NAT	2.07	1.44	1.38
4	D	1000	4KU	CAV-NAT	2.07	1.44	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1000	4KU	CAR-CAQ-CAW	-8.22	99.98	112.77
4	A	1000	4KU	CAO-CAY-CAW	-5.90	117.80	121.79
4	B	1000	4KU	CAO-CAY-CAW	-5.22	118.25	121.79
4	C	1000	4KU	CAR-CAQ-CAW	-4.74	105.39	112.77
4	C	1000	4KU	CAO-CAY-CAW	-4.59	118.68	121.79
4	B	1000	4KU	CAR-CAQ-CAW	-4.46	105.83	112.77
4	A	1000	4KU	CAP-CAZ-CAX	-4.44	118.78	121.79
4	D	1000	4KU	CAR-CAQ-CAW	-4.39	105.94	112.77
4	D	1000	4KU	CAO-CAY-CAW	-3.91	119.14	121.79
4	C	1000	4KU	CAP-CAZ-CAX	-3.49	119.42	121.79
4	B	1000	4KU	CAP-CAZ-CAX	-3.12	119.68	121.79
4	D	1000	4KU	CAP-CAZ-CAX	-2.75	119.93	121.79
4	A	1000	4KU	CAL-CAN-CAX	-2.65	117.82	121.41
4	C	1000	4KU	CAL-CAN-CAX	-2.37	118.21	121.41
4	B	1000	4KU	CAL-CAN-CAX	-2.32	118.28	121.41
4	D	1000	4KU	CAL-CAN-CAX	-2.29	118.31	121.41
4	B	1000	4KU	CAU-CAO-CAY	2.10	121.44	119.28
4	B	1000	4KU	CAO-CAY-SBA	2.10	121.30	117.28
4	A	1000	4KU	CAQ-CAR-CAX	2.29	116.33	112.77
4	D	1000	4KU	CAM-CAW-CAY	2.32	119.69	116.04
4	A	1000	4KU	CAM-CAW-CAY	2.60	120.13	116.04
4	B	1000	4KU	CAM-CAW-CAY	2.82	120.48	116.04
4	D	1000	4KU	CAN-CAX-CAZ	2.82	120.48	116.04
4	A	1000	4KU	CAU-CAO-CAY	2.84	122.20	119.28
4	B	1000	4KU	CAN-CAX-CAZ	3.03	120.80	116.04
4	C	1000	4KU	CAM-CAW-CAY	3.05	120.83	116.04
4	C	1000	4KU	CAN-CAX-CAZ	3.23	121.12	116.04
4	A	1000	4KU	CAN-CAX-CAZ	3.66	121.79	116.04
4	A	1000	4KU	OAA-SBA-CAY	4.34	111.17	106.17
4	B	1000	4KU	OAD-SBB-CAZ	5.04	111.98	106.17
4	C	1000	4KU	OAF-SBB-CAZ	5.35	112.33	106.17
4	C	1000	4KU	OAA-SBA-CAY	5.52	112.54	106.17
4	A	1000	4KU	OAF-SBB-CAZ	5.62	112.65	106.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1000	4KU	OAD-SBB-CAZ	5.67	112.70	106.17
4	D	1000	4KU	OAF-SBB-CAZ	6.98	114.21	106.17
4	B	1000	4KU	OAA-SBA-CAY	7.31	114.60	106.17
4	D	1000	4KU	OAB-SBA-CAY	7.43	114.73	106.17
4	C	1000	4KU	OAB-SBA-CAY	7.46	114.77	106.17
4	D	1000	4KU	OAA-SBA-CAY	7.60	114.93	106.17
4	B	1000	4KU	OAF-SBB-CAZ	7.71	115.06	106.17
4	C	1000	4KU	OAD-SBB-CAZ	7.97	115.36	106.17
4	B	1000	4KU	OAB-SBA-CAY	8.51	115.97	106.17
4	A	1000	4KU	OAD-SBB-CAZ	9.55	117.18	106.17
4	A	1000	4KU	OAB-SBA-CAY	10.00	117.69	106.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	4KU	1	0
4	B	1000	4KU	2	0
4	C	1000	4KU	3	0
4	D	1000	4KU	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	475/911 (52%)	-0.20	12 (2%) 61 50	71, 103, 169, 208	0
1	B	475/911 (52%)	-0.03	28 (5%) 26 20	90, 142, 202, 249	0
1	C	475/911 (52%)	-0.16	13 (2%) 58 47	79, 114, 184, 226	0
1	D	475/911 (52%)	-0.02	24 (5%) 32 24	103, 151, 219, 259	0
2	E	223/223 (100%)	0.30	23 (10%) 9 8	79, 105, 150, 177	0
2	G	223/223 (100%)	0.26	19 (8%) 13 12	124, 152, 211, 250	0
2	I	223/223 (100%)	1.13	41 (18%) 2 2	79, 112, 310, 355	0
2	K	223/223 (100%)	0.30	17 (7%) 17 14	126, 152, 209, 248	0
3	F	218/218 (100%)	0.11	19 (8%) 13 12	81, 111, 141, 179	0
3	H	218/218 (100%)	0.84	49 (22%) 1 1	125, 181, 255, 268	0
3	J	218/218 (100%)	0.83	43 (19%) 1 2	90, 164, 292, 310	0
3	L	218/218 (100%)	0.52	31 (14%) 4 4	127, 169, 242, 253	0
All	All	3664/5408 (67%)	0.20	319 (8%) 13 12	71, 139, 238, 355	0

All (319) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	143	GLY	18.2
2	I	135	ALA	17.2
2	I	195	SER	14.6
2	I	144	SER	13.2
2	I	140	ASP	11.3
3	J	135	SER	10.3
2	K	141	THR	10.1
3	H	216	ASN	9.7
2	K	140	ASP	9.6
3	F	194	ASN	9.5
2	I	167	GLY	9.5

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Mol	Chain	Res	Type	RSRZ
3	J	136	VAL	9.0
2	I	170	SER	8.9
2	I	163	THR	8.8
2	I	194	THR	8.8
3	J	184	THR	8.6
2	G	139	GLY	7.9
3	L	216	ASN	7.4
3	J	175	SER	6.9
2	I	161	THR	6.4
2	I	145	SER	6.3
2	I	168	SER	6.1
2	K	139	GLY	6.1
2	I	196	SER	6.1
2	I	139	GLY	5.9
3	J	162	GLY	5.8
2	G	140	ASP	5.8
2	I	162	LEU	5.8
2	G	137	VAL	5.7
1	A	819	HIS	5.7
2	I	148	LEU	5.7
2	I	141	THR	5.6
3	H	174	ASP	5.6
3	J	134	ALA	5.6
2	K	183	ASP	5.6
3	J	183	LEU	5.5
2	G	200	SER	5.5
2	E	195	SER	5.5
2	I	147	THR	5.5
2	E	196	SER	5.3
3	J	172	SER	5.3
3	J	137	VAL	5.2
3	H	218	CYS	5.2
2	I	166	SER	5.2
2	I	193	VAL	5.2
2	I	136	PRO	5.1
2	I	169	LEU	5.0
1	D	874	LEU	5.0
2	G	138	CYS	5.0
1	C	818	TYR	5.0
3	J	173	LYS	4.9
2	G	141	THR	4.9
3	L	155	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
3	L	218	CYS	4.8
3	L	146	LYS	4.8
2	I	142	THR	4.8
1	B	755	GLU	4.7
2	I	223	ARG	4.7
3	J	124	PRO	4.7
1	B	649	VAL	4.6
2	K	31	THR	4.6
3	J	193	HIS	4.6
1	C	398	THR	4.6
3	J	128	GLN	4.5
2	G	222	PRO	4.5
3	H	213	PHE	4.5
3	H	176	THR	4.5
2	E	154	GLY	4.4
3	H	121	ILE	4.4
3	H	112	ARG	4.4
1	A	831	TRP	4.4
3	H	142	ASN	4.3
1	B	818	TYR	4.3
2	G	136	PRO	4.2
1	D	834	HIS	4.2
3	F	193	HIS	4.2
3	F	206	THR	4.2
3	H	173	LYS	4.1
2	I	138	CYS	4.1
1	D	866	THR	4.1
1	D	870	ARG	4.1
2	I	208	ALA	4.1
3	H	210	VAL	4.0
3	J	160	GLN	4.0
3	L	124	PRO	4.0
1	B	754	GLN	4.0
1	A	398	THR	4.0
1	B	653	LEU	4.0
3	L	37	MET	3.9
3	H	36	TYR	3.9
1	B	639	LYS	3.9
1	D	700	SER	3.9
1	A	832	ARG	3.8
3	H	212	SER	3.8
2	G	148	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	I	187	LEU	3.8
3	J	122	PHE	3.8
2	K	142	THR	3.7
1	A	830	THR	3.7
3	J	121	ILE	3.7
3	H	35	SER	3.7
1	C	819	HIS	3.7
3	J	194	ASN	3.7
1	B	875	PRO	3.6
3	L	131	SER	3.6
2	I	165	ASN	3.6
3	H	39	TRP	3.6
3	H	191	GLU	3.6
3	L	217	GLU	3.5
3	J	185	LEU	3.5
1	B	821	ASP	3.5
3	J	120	SER	3.5
2	I	146	VAL	3.5
2	I	206	ASN	3.5
3	H	119	VAL	3.5
3	L	55	ALA	3.5
3	L	36	TYR	3.5
2	I	201	GLN	3.5
3	L	154	ILE	3.5
2	E	220	ILE	3.4
2	G	202	SER	3.4
2	K	170	SER	3.4
3	L	39	TRP	3.4
3	F	19	ALA	3.4
1	A	816	PRO	3.4
3	H	211	LYS	3.4
2	G	174	HIS	3.4
3	H	214	ASN	3.4
3	J	191	GLU	3.3
1	B	874	LEU	3.3
1	B	695	LYS	3.3
3	H	187	LYS	3.3
3	J	12	ALA	3.3
1	A	553	TYR	3.3
3	L	184	THR	3.3
3	J	81	PRO	3.2
3	J	11	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	817	LYS	3.2
2	I	207	VAL	3.2
3	F	216	ASN	3.2
3	J	161	ASN	3.2
3	L	129	LEU	3.2
3	L	132	GLY	3.2
1	B	870	ARG	3.1
3	H	207	SER	3.1
3	J	139	PHE	3.1
1	B	650	ILE	3.1
2	I	215	LYS	3.1
2	K	148	LEU	3.1
3	J	215	ARG	3.1
2	G	221	GLU	3.1
1	D	837	THR	3.1
1	D	835	LEU	3.1
1	B	654	GLY	3.1
2	E	149	GLY	3.1
1	D	755	GLU	3.1
3	J	119	VAL	3.0
3	H	63	PRO	3.0
3	J	154	ILE	3.0
1	C	821	ASP	3.0
1	C	817	LYS	3.0
2	E	107	GLY	3.0
3	H	66	PHE	3.0
2	E	183	ASP	3.0
3	H	55	ALA	3.0
1	D	398	THR	3.0
2	E	194	THR	3.0
3	L	203	LYS	3.0
3	F	215	ARG	3.0
2	E	122	SER	3.0
3	J	170	GLN	3.0
1	B	872	VAL	3.0
3	H	134	ALA	3.0
1	D	819	HIS	2.9
3	J	207	SER	2.9
2	I	197	THR	2.9
3	F	203	LYS	2.9
1	D	519	TYR	2.9
3	H	190	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
3	L	185	LEU	2.8
2	E	144	SER	2.8
1	D	869	LEU	2.8
3	H	171	ASP	2.8
1	C	400	ALA	2.8
3	F	217	GLU	2.8
3	L	133	GLY	2.8
2	E	153	LYS	2.8
3	J	84	GLU	2.8
2	E	108	TYR	2.8
3	H	60	SER	2.8
2	I	186	THR	2.8
3	F	214	ASN	2.8
1	D	387	ARG	2.7
3	H	133	GLY	2.7
1	B	820	PRO	2.7
2	E	181	GLN	2.7
3	F	79	ILE	2.7
1	B	651	HIS	2.7
3	L	165	ASN	2.7
3	J	43	LYS	2.7
1	D	649	VAL	2.7
1	C	835	LEU	2.7
1	C	831	TRP	2.7
2	G	142	THR	2.7
3	L	63	PRO	2.6
3	J	123	PRO	2.6
1	D	839	ILE	2.6
3	F	207	SER	2.6
1	B	601	LEU	2.6
2	K	181	GLN	2.6
2	G	201	GLN	2.6
3	J	85	GLU	2.6
3	H	185	LEU	2.6
2	E	180	LEU	2.6
3	H	129	LEU	2.6
2	G	219	LYS	2.6
2	E	14	PRO	2.6
2	K	71	ILE	2.6
2	I	171	SER	2.6
1	A	834	HIS	2.5
3	J	216	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	198	TRP	2.5
2	I	217	ASP	2.5
2	E	221	GLU	2.5
2	E	123	SER	2.5
3	F	18	ARG	2.5
3	H	54	TYR	2.5
3	H	130	THR	2.5
2	I	164	TRP	2.5
3	J	112	ARG	2.5
1	D	650	ILE	2.5
2	E	1	GLU	2.5
1	B	638	PHE	2.5
3	L	4	MET	2.5
3	F	17	GLN	2.5
1	B	640	VAL	2.5
3	J	97	GLU	2.5
3	J	67	SER	2.5
1	B	839	ILE	2.5
3	L	134	ALA	2.5
1	B	819	HIS	2.5
1	B	394	LEU	2.4
1	D	876	LEU	2.4
3	H	124	PRO	2.4
1	C	397	ILE	2.4
2	G	122	SER	2.4
3	H	116	ALA	2.4
3	J	131	SER	2.4
1	D	754	GLN	2.4
3	J	83	GLU	2.4
2	K	138	CYS	2.4
2	G	220	ILE	2.4
1	D	693	GLU	2.3
2	K	169	LEU	2.3
3	L	196	TYR	2.3
3	H	126	SER	2.3
3	L	147	ASP	2.3
1	D	873	LEU	2.3
1	B	652	PRO	2.3
1	D	652	PRO	2.3
3	F	189	GLU	2.3
2	I	200	SER	2.3
2	I	192	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	H	175	SER	2.3
2	G	135	ALA	2.3
2	G	31	THR	2.3
2	I	179	VAL	2.3
1	B	886	LEU	2.3
3	H	215	ARG	2.3
2	K	179	VAL	2.3
3	H	209	ILE	2.3
3	H	196	TYR	2.3
1	B	637	GLY	2.3
3	H	64	ALA	2.3
3	J	125	SER	2.2
2	K	137	VAL	2.2
3	H	141	ASN	2.2
1	C	816	PRO	2.2
1	C	625	GLN	2.2
3	L	130	THR	2.2
3	H	38	ASN	2.2
2	E	148	LEU	2.2
3	H	115	ALA	2.2
2	E	197	THR	2.2
3	L	56	SER	2.2
2	E	143	GLY	2.2
3	H	172	SER	2.2
1	B	836	PHE	2.2
3	F	208	PRO	2.1
3	F	192	ARG	2.1
3	J	210	VAL	2.1
1	D	412	ILE	2.1
3	H	68	GLY	2.1
2	K	182	SER	2.1
2	K	134	LEU	2.1
3	H	155	ASP	2.1
3	L	114	ASP	2.1
3	J	171	ASP	2.1
1	A	873	LEU	2.1
1	B	866	THR	2.1
3	F	51	LEU	2.1
3	F	161	ASN	2.1
3	H	200	ALA	2.1
3	L	193	HIS	2.1
3	L	62	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	128	GLN	2.1
1	D	654	GLY	2.1
1	C	834	HIS	2.0
2	E	145	SER	2.0
1	A	818	TYR	2.0
1	B	871	ARG	2.0
1	C	401	PHE	2.0
3	F	195	SER	2.0
3	H	205	SER	2.0
3	L	125	SER	2.0
3	H	84	GLU	2.0
1	A	835	LEU	2.0
2	K	124	ALA	2.0
1	D	655	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	4KU	C	1000	28/28	0.76	0.32	1.21	113,118,123,125	0
4	4KU	A	1000	28/28	0.78	0.29	0.27	105,108,112,114	0
4	4KU	B	1000	28/28	0.80	0.27	-0.13	143,146,152,155	0
4	4KU	D	1000	28/28	0.81	0.25	-0.21	148,152,159,163	0

6.5 Other polymers (i)

There are no such residues in this entry.