



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:53 PM GMT

PDB ID : 4N0F
Title : Human FcRn complexed with human serum albumin
Authors : Oganessian, V.; Wu, H.; Dall'Acqua, W.F.
Deposited on : 2013-10-01
Resolution : 3.02 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

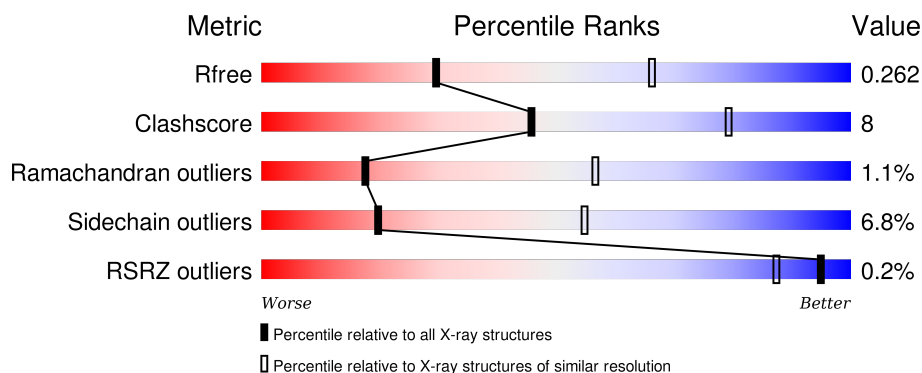
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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 $\leq 5\%$. 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	271	<div> <div></div> <div>77%18% . .</div> </div>
1	E	271	<div> <div></div> <div>74%20% . .</div> </div>
1	H	271	<div> <div>%</div> <div>73%20% . .</div> </div>
1	K	271	<div> <div></div> <div>76%18% . .</div> </div>
2	B	99	<div> <div></div> <div>82%16% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	99	<div><div></div><div>78%21%</div><div></div></div>
2	I	99	<div><div></div><div>%88%11%</div><div></div></div>
2	L	99	<div><div></div><div>86%12%</div><div></div></div>
3	D	585	<div><div></div><div>80%17%</div><div></div></div>
3	G	585	<div><div></div><div>78%19%</div><div></div></div>
3	J	585	<div><div></div><div>78%19%</div><div></div></div>
3	M	585	<div><div></div><div>81%16%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30181 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2079	1330	360	381	8			
1	E	264	Total	C	N	O	S	0	0	0
			2079	1330	360	381	8			
1	H	264	Total	C	N	O	S	0	0	0
			2079	1330	360	381	8			
1	K	264	Total	C	N	O	S	0	0	0
			2079	1330	360	381	8			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	F	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	I	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	L	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

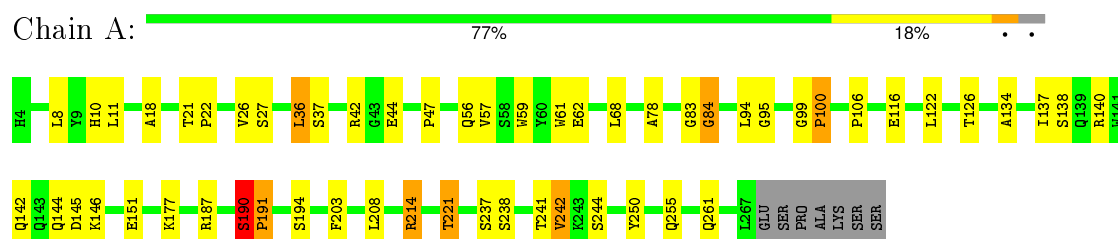
- Molecule 3 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	583	Total	C	N	O	S	0	0	0
			4638	2929	784	884	41			
3	G	583	Total	C	N	O	S	0	0	0
			4638	2929	784	884	41			
3	J	583	Total	C	N	O	S	0	0	0
			4638	2929	784	884	41			
3	M	583	Total	C	N	O	S	0	0	0
			4638	2929	784	884	41			

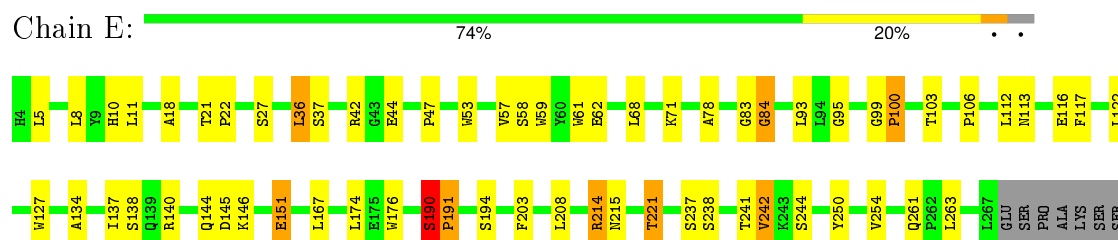
3 Residue-property plots [i](#)

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.

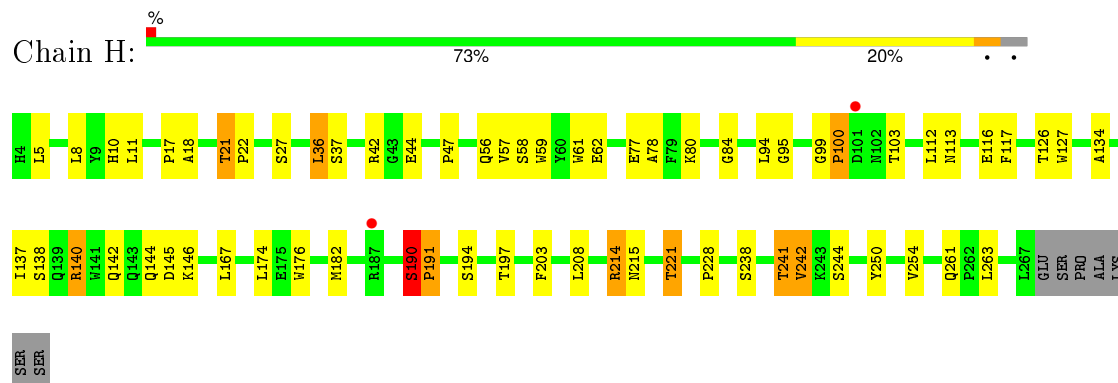
- Molecule 1: IgG receptor FcRn large subunit p51



- Molecule 1: IgG receptor FcRn large subunit p51

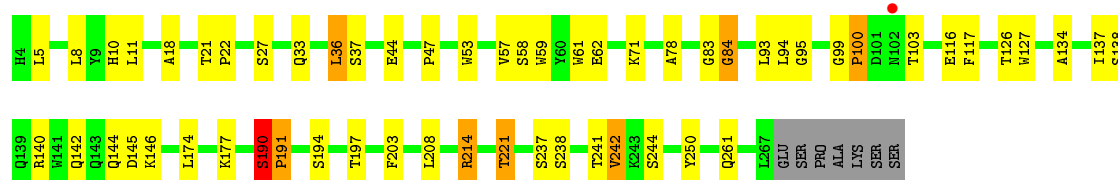


- Molecule 1: IgG receptor FcRn large subunit p51

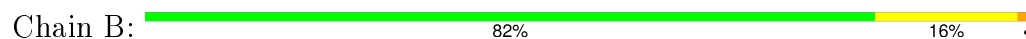


- Molecule 1: IgG receptor FcRn large subunit p51

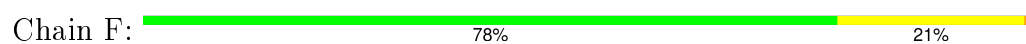




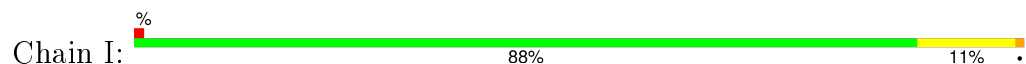
• Molecule 2: Beta-2-microglobulin



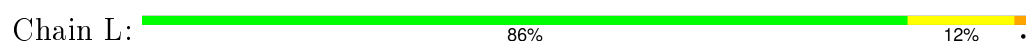
• Molecule 2: Beta-2-microglobulin



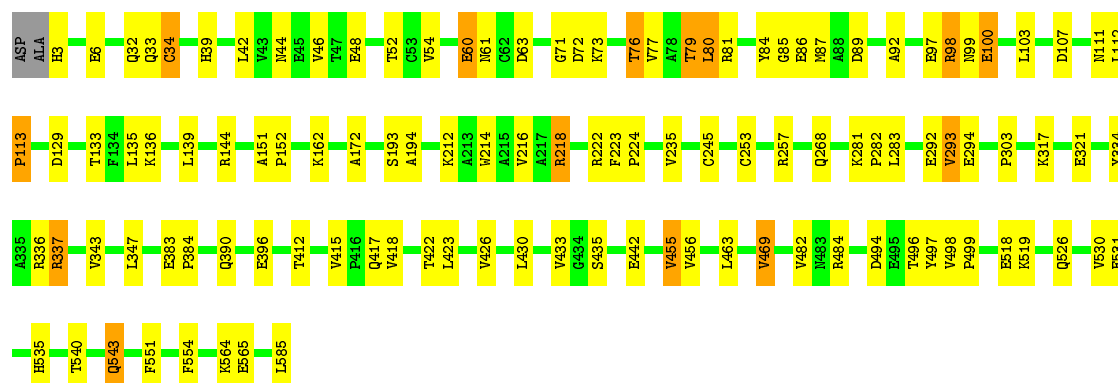
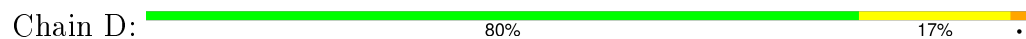
• Molecule 2: Beta-2-microglobulin




• Molecule 2: Beta-2-microglobulin

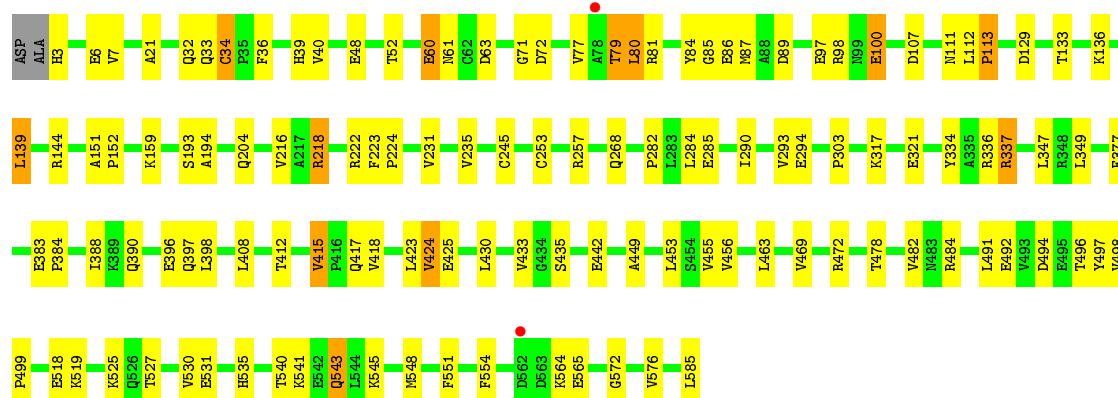


• Molecule 3: Serum albumin




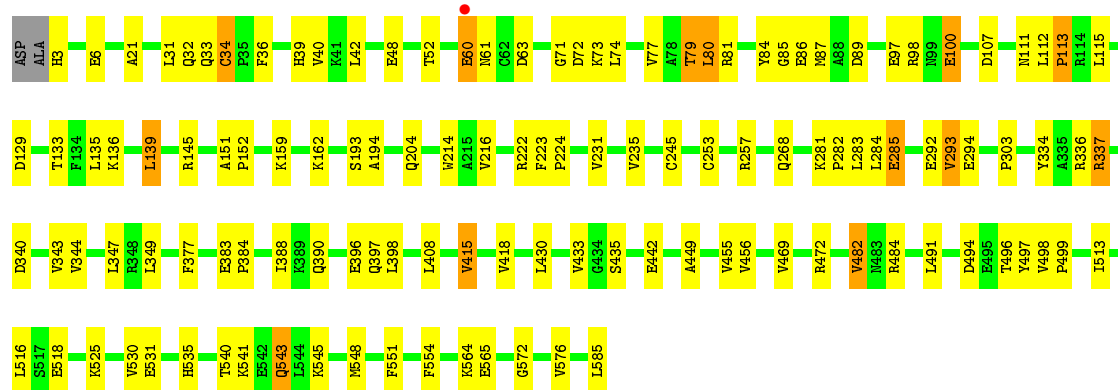
• Molecule 3: Serum albumin

Chain G:  78% 19%




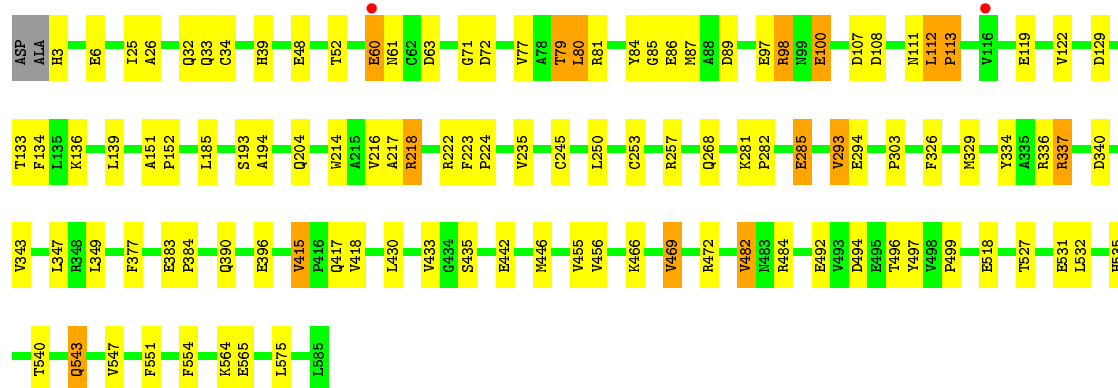
• Molecule 3: Serum albumin

Chain J:  78% 19%



• Molecule 3: Serum albumin

Chain M:  81% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.47Å 115.92Å 186.24Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	20.00 – 3.02 44.26 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.02) 99.2 (44.26-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.260 0.227 , 0.262	Depositor DCC
R_{free} test set	5480 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	7 of 109961 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30181	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 48.74 % 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 8.2461e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 ⓘ

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	0.79	1/2145 (0.0%)	0.81	0/2915
1	E	0.80	3/2145 (0.1%)	0.81	0/2915
1	H	0.79	2/2145 (0.1%)	0.79	1/2915 (0.0%)
1	K	0.80	1/2145 (0.0%)	0.78	0/2915
2	B	0.72	1/851 (0.1%)	0.76	1/1152 (0.1%)
2	F	0.68	0/851	0.73	0/1152
2	I	0.63	0/851	0.71	0/1152
2	L	0.65	0/852	0.69	0/1152
3	D	0.63	0/4728	0.77	1/6377 (0.0%)
3	G	0.65	0/4728	0.77	1/6377 (0.0%)
3	J	0.63	0/4728	0.76	1/6377 (0.0%)
3	M	0.62	0/4728	0.77	4/6377 (0.1%)
All	All	0.69	8/30897 (0.0%)	0.77	9/41776 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	151	GLU	CD-OE2	6.67	1.32	1.25
1	A	151	GLU	CD-OE2	6.43	1.32	1.25
1	H	127	TRP	CD2-CE2	5.40	1.47	1.41
1	H	176	TRP	CD2-CE2	5.29	1.47	1.41
2	B	95	TRP	CD2-CE2	5.28	1.47	1.41
1	E	127	TRP	CD2-CE2	5.05	1.47	1.41
1	K	127	TRP	CD2-CE2	5.02	1.47	1.41
1	E	176	TRP	CD2-CE2	5.00	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	340	ASP	CB-CG-OD2	7.52	125.07	118.30
2	B	45	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	H	190	SER	CB-CA-C	5.77	121.06	110.10
3	M	63	ASP	CB-CG-OD2	5.68	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	63	ASP	CB-CG-OD1	-5.56	113.29	118.30
3	G	218	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	M	218	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	D	218	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	M	340	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2079	0	1990	40	0
1	E	2079	0	1990	41	0
1	H	2079	0	1990	51	0
1	K	2079	0	1990	39	0
2	B	828	0	794	8	0
2	F	828	0	794	8	0
2	I	828	0	794	7	0
2	L	829	0	794	6	0
3	D	4638	0	4563	75	0
3	G	4638	0	4563	75	0
3	J	4638	0	4563	78	0
3	M	4638	0	4563	63	0
All	All	30181	0	29388	459	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 8.

All (459) 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)
3:D:33:GLN:HE21	3:D:112:LEU:CD1	1.59	1.16
3:M:112:LEU:HD23	3:M:113:PRO:HD2	1.29	1.08
3:J:33:GLN:HE21	3:J:112:LEU:CD1	1.71	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:CD1	1:A:94:LEU:HD13	1.91	1.00
3:D:33:GLN:HE21	3:D:112:LEU:HD11	1.29	0.97
3:J:33:GLN:NE2	3:J:112:LEU:HD11	1.79	0.96
3:J:33:GLN:HE21	3:J:112:LEU:HD11	1.30	0.96
3:J:115:LEU:HB2	3:J:145:ARG:HH12	1.28	0.95
1:A:11:LEU:HD13	1:A:94:LEU:HD13	1.50	0.94
3:J:33:GLN:NE2	3:J:112:LEU:CD1	2.35	0.87
3:G:430:LEU:HD23	3:G:456:VAL:HG11	1.54	0.87
1:A:57:VAL:HG11	3:D:111:ASN:HB3	1.58	0.84
3:M:112:LEU:HD23	3:M:113:PRO:CD	2.08	0.83
3:D:430:LEU:HD23	3:D:456:VAL:HG11	1.58	0.83
3:D:33:GLN:NE2	3:D:112:LEU:CD1	2.41	0.82
3:J:115:LEU:CB	3:J:145:ARG:HH12	1.93	0.81
3:G:33:GLN:HE21	3:G:112:LEU:CD1	1.93	0.81
2:B:83:ASN:HD22	2:B:84:HIS:H	1.27	0.79
3:M:151:ALA:HB3	3:M:152:PRO:HD3	1.65	0.78
2:L:83:ASN:HD22	2:L:84:HIS:H	1.32	0.75
1:A:36:LEU:HD23	1:A:37:SER:N	2.02	0.74
1:A:44:GLU:HG3	3:D:417:GLN:NE2	2.03	0.74
3:J:151:ALA:HB3	3:J:152:PRO:HD3	1.70	0.74
3:J:194:ALA:HB1	3:J:455:VAL:CG1	2.17	0.74
1:H:8:LEU:HD23	1:H:95:GLY:HA3	1.68	0.74
1:K:144:GLN:O	1:K:146:LYS:N	2.21	0.74
3:J:77:VAL:O	3:J:80:LEU:HG	1.89	0.73
3:D:33:GLN:HE21	3:D:112:LEU:HD12	1.51	0.73
3:G:151:ALA:HB3	3:G:152:PRO:HD3	1.69	0.73
3:J:115:LEU:HB2	3:J:145:ARG:NH1	2.03	0.73
3:D:77:VAL:O	3:D:80:LEU:HG	1.89	0.73
3:M:77:VAL:O	3:M:80:LEU:HG	1.89	0.72
3:D:151:ALA:HB3	3:D:152:PRO:HD3	1.72	0.72
1:E:144:GLN:O	1:E:146:LYS:N	2.22	0.72
1:A:144:GLN:O	1:A:146:LYS:N	2.22	0.72
1:A:18:ALA:O	1:A:21:THR:HB	1.91	0.70
3:J:430:LEU:HD23	3:J:456:VAL:HG11	1.72	0.70
3:G:430:LEU:CD2	3:G:456:VAL:HG11	2.22	0.69
2:L:83:ASN:HD22	2:L:84:HIS:N	1.89	0.69
3:G:77:VAL:O	3:G:80:LEU:HG	1.92	0.69
1:H:78:ALA:HB1	1:H:137:ILE:HD13	1.73	0.69
3:D:33:GLN:NE2	3:D:112:LEU:HD11	2.06	0.68
1:H:144:GLN:O	1:H:146:LYS:N	2.23	0.68
2:I:2:GLN:HE22	2:I:85:VAL:HG11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:83:ASN:HD22	2:I:84:HIS:H	1.40	0.67
3:M:194:ALA:HB1	3:M:455:VAL:CG1	2.24	0.67
3:J:33:GLN:HE21	3:J:112:LEU:HD13	1.55	0.67
3:G:33:GLN:NE2	3:G:112:LEU:CD1	2.58	0.66
1:E:18:ALA:O	1:E:21:THR:HB	1.95	0.66
1:H:18:ALA:O	1:H:21:THR:HB	1.96	0.66
1:K:18:ALA:O	1:K:21:THR:HB	1.96	0.66
1:A:11:LEU:HD13	1:A:94:LEU:CD1	2.25	0.66
1:E:241:THR:O	1:E:242:VAL:HG23	1.97	0.65
3:M:430:LEU:HD23	3:M:456:VAL:HG11	1.78	0.65
1:H:11:LEU:HD12	1:H:11:LEU:H	1.61	0.65
2:B:83:ASN:HD22	2:B:84:HIS:N	1.95	0.65
1:A:36:LEU:C	1:A:36:LEU:HD23	2.17	0.65
1:K:57:VAL:HG11	3:M:111:ASN:HB3	1.78	0.64
1:E:36:LEU:HD23	1:E:37:SER:N	2.12	0.64
3:M:81:ARG:NH2	3:M:89:ASP:OD2	2.31	0.64
1:K:36:LEU:HD23	1:K:37:SER:N	2.12	0.64
3:G:36:PHE:O	3:G:40:VAL:HG23	1.97	0.63
3:D:216:VAL:HG22	3:D:235:VAL:HG21	1.80	0.63
3:J:81:ARG:NH2	3:J:89:ASP:OD2	2.31	0.63
3:D:33:GLN:NE2	3:D:112:LEU:HD12	2.12	0.63
1:E:57:VAL:HG11	3:G:111:ASN:HB3	1.80	0.63
1:E:57:VAL:HG11	3:G:111:ASN:CG	2.19	0.62
3:J:415:VAL:CG1	3:J:415:VAL:O	2.48	0.62
3:G:540:THR:H	3:G:543:GLN:HE21	1.48	0.62
1:K:44:GLU:CD	3:M:469:VAL:HG22	2.20	0.62
3:D:430:LEU:CD2	3:D:456:VAL:HG11	2.30	0.62
3:D:81:ARG:NH2	3:D:89:ASP:OD2	2.32	0.62
3:D:415:VAL:CG1	3:D:415:VAL:O	2.48	0.62
3:M:347:LEU:HB2	3:M:482:VAL:HG21	1.82	0.62
3:J:415:VAL:HG13	3:J:418:VAL:HG23	1.82	0.62
1:K:47:PRO:HB3	1:K:61:TRP:CZ2	2.35	0.62
3:G:81:ARG:NH2	3:G:89:ASP:OD2	2.32	0.61
3:M:79:THR:O	3:M:81:ARG:N	2.34	0.61
2:L:24:ASN:HB3	2:L:65:LEU:HD11	1.83	0.61
1:H:47:PRO:HB3	1:H:61:TRP:CZ2	2.36	0.61
3:J:34:CYS:N	3:J:84:TYR:OH	2.34	0.61
3:G:415:VAL:HG13	3:G:418:VAL:HG23	1.82	0.61
1:H:11:LEU:CD1	1:H:94:LEU:HD12	2.29	0.61
3:G:347:LEU:HB2	3:G:482:VAL:HG21	1.83	0.61
3:J:540:THR:H	3:J:543:GLN:HE21	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:MET:CE	1:H:254:VAL:HB	2.31	0.60
1:K:57:VAL:HG11	3:M:111:ASN:CB	2.30	0.60
3:M:415:VAL:CG1	3:M:415:VAL:O	2.50	0.60
1:E:11:LEU:H	1:E:11:LEU:HD12	1.66	0.60
3:M:34:CYS:N	3:M:84:TYR:OH	2.35	0.60
3:D:79:THR:O	3:D:81:ARG:N	2.34	0.59
3:J:541:LYS:NZ	3:J:545:LYS:HE3	2.17	0.59
3:D:540:THR:H	3:D:543:GLN:HE21	1.51	0.59
3:J:216:VAL:CG2	3:J:235:VAL:HG21	2.32	0.59
3:J:216:VAL:HG22	3:J:235:VAL:HG21	1.84	0.59
1:E:57:VAL:HG11	3:G:111:ASN:CB	2.32	0.59
3:J:79:THR:O	3:J:81:ARG:N	2.36	0.59
2:F:83:ASN:HD22	2:F:84:HIS:H	1.49	0.59
1:K:93:LEU:O	1:K:94:LEU:HD23	2.02	0.59
1:A:57:VAL:HG11	3:D:111:ASN:CB	2.30	0.58
3:D:60:GLU:O	3:D:61:ASN:HB2	2.02	0.58
1:E:47:PRO:HB3	1:E:61:TRP:CZ2	2.38	0.58
1:K:11:LEU:H	1:K:11:LEU:HD12	1.68	0.58
3:J:194:ALA:HB1	3:J:455:VAL:HG11	1.84	0.58
3:M:194:ALA:HB1	3:M:455:VAL:HG13	1.86	0.58
1:E:21:THR:HG23	1:E:22:PRO:HD2	1.86	0.58
3:G:79:THR:O	3:G:81:ARG:N	2.36	0.58
3:G:33:GLN:NE2	3:G:112:LEU:HD11	2.18	0.58
3:G:34:CYS:N	3:G:84:TYR:OH	2.36	0.58
3:D:34:CYS:N	3:D:84:TYR:OH	2.35	0.58
1:H:36:LEU:HD23	1:H:37:SER:N	2.18	0.58
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.39	0.58
3:G:218:ARG:HG2	3:G:218:ARG:HH11	1.69	0.58
3:D:218:ARG:HH11	3:D:218:ARG:HG2	1.69	0.57
1:H:182:MET:HE2	1:H:254:VAL:HG11	1.85	0.57
3:J:194:ALA:HB1	3:J:455:VAL:HG13	1.84	0.57
3:G:541:LYS:HZ2	3:G:545:LYS:HE3	1.68	0.57
1:E:78:ALA:HB1	1:E:137:ILE:HD13	1.86	0.57
3:D:293:VAL:HG22	3:D:294:GLU:H	1.69	0.57
3:M:60:GLU:O	3:M:61:ASN:HB2	2.05	0.57
3:M:218:ARG:HG2	3:M:218:ARG:HH11	1.68	0.56
3:G:531:GLU:O	3:G:535:HIS:HD2	1.88	0.56
1:K:57:VAL:HG12	1:K:58:SER:O	2.05	0.56
2:I:2:GLN:HE22	2:I:85:VAL:CG1	2.18	0.56
1:E:71:LYS:NZ	1:E:151:GLU:OE1	2.28	0.56
3:D:415:VAL:HG13	3:D:418:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:VAL:HG11	3:J:111:ASN:HB3	1.87	0.56
1:E:57:VAL:HG12	1:E:58:SER:N	2.21	0.56
1:H:11:LEU:HD11	1:H:94:LEU:HD12	1.88	0.56
1:K:33:GLN:NE2	1:K:174:LEU:HD23	2.20	0.56
3:J:80:LEU:O	3:J:84:TYR:N	2.39	0.55
3:J:159:LYS:CE	3:J:284:LEU:HD12	2.36	0.55
3:G:388:ILE:HD13	3:G:449:ALA:CB	2.36	0.55
3:G:216:VAL:HG22	3:G:235:VAL:HG21	1.87	0.55
3:M:80:LEU:O	3:M:84:TYR:N	2.40	0.55
3:D:417:GLN:HA	3:D:417:GLN:OE1	2.05	0.55
1:K:214:ARG:HG3	1:K:250:TYR:CZ	2.42	0.55
3:G:33:GLN:HE21	3:G:112:LEU:HD11	1.69	0.55
3:J:293:VAL:HG22	3:J:294:GLU:H	1.71	0.54
3:M:531:GLU:O	3:M:535:HIS:HD2	1.90	0.54
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.89	0.54
3:D:80:LEU:O	3:D:84:TYR:N	2.40	0.54
3:G:60:GLU:O	3:G:61:ASN:HB2	2.07	0.54
3:J:347:LEU:HB2	3:J:482:VAL:HG21	1.89	0.54
1:K:190:SER:OG	1:K:191:PRO:HD2	2.08	0.54
3:G:541:LYS:NZ	3:G:545:LYS:HE3	2.23	0.54
3:D:347:LEU:HB2	3:D:482:VAL:HG21	1.88	0.54
1:K:21:THR:HG23	1:K:22:PRO:HD2	1.89	0.54
1:H:182:MET:HE2	1:H:254:VAL:CG1	2.38	0.54
2:F:2:GLN:NE2	2:F:85:VAL:HG11	2.23	0.54
1:A:203:PHE:CZ	1:A:208:LEU:HD13	2.43	0.54
3:D:531:GLU:O	3:D:535:HIS:HD2	1.91	0.53
3:J:48:GLU:O	3:J:52:THR:HG23	2.07	0.53
3:J:60:GLU:O	3:J:61:ASN:HB2	2.08	0.53
1:A:190:SER:OG	1:A:191:PRO:HD2	2.09	0.53
1:K:208:LEU:HD23	1:K:208:LEU:C	2.29	0.53
1:E:190:SER:OG	1:E:191:PRO:HD2	2.08	0.53
1:A:21:THR:HG23	1:A:22:PRO:HD2	1.91	0.53
3:G:80:LEU:O	3:G:84:TYR:N	2.40	0.53
3:G:194:ALA:HB1	3:G:455:VAL:CG1	2.38	0.53
3:D:214:TRP:CD1	3:D:343:VAL:HG11	2.44	0.53
1:E:134:ALA:O	1:E:138:SER:HB2	2.09	0.53
1:H:190:SER:OG	1:H:191:PRO:HD2	2.09	0.53
1:H:221:THR:HG22	1:H:238:SER:OG	2.08	0.53
3:M:282:PRO:HG2	3:M:285:GLU:HG3	1.91	0.53
3:M:48:GLU:O	3:M:52:THR:HG23	2.07	0.53
3:D:112:LEU:HD21	3:D:144:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:282:PRO:HG2	3:J:285:GLU:HG3	1.91	0.52
3:G:424:VAL:HG12	3:G:425:GLU:N	2.23	0.52
3:G:159:LYS:HE2	3:G:284:LEU:HD12	1.91	0.52
3:J:531:GLU:O	3:J:535:HIS:HD2	1.93	0.52
1:A:134:ALA:O	1:A:138:SER:HB2	2.10	0.52
2:L:37:VAL:HB	2:L:66:TYR:CE1	2.45	0.52
3:M:224:PRO:O	3:M:336:ARG:NH1	2.42	0.52
1:H:182:MET:HE2	1:H:254:VAL:HB	1.92	0.52
1:E:36:LEU:C	1:E:36:LEU:HD23	2.31	0.51
1:K:134:ALA:O	1:K:138:SER:HB2	2.10	0.51
3:J:224:PRO:O	3:J:336:ARG:NH1	2.43	0.51
3:M:216:VAL:HG22	3:M:235:VAL:HG21	1.92	0.51
3:G:282:PRO:HG2	3:G:285:GLU:HG3	1.92	0.51
3:G:415:VAL:HG13	3:G:418:VAL:CG2	2.40	0.51
1:H:134:ALA:O	1:H:138:SER:HB2	2.10	0.51
1:K:221:THR:HG22	1:K:238:SER:OG	2.10	0.51
3:M:216:VAL:CG2	3:M:235:VAL:HG21	2.41	0.51
1:A:214:ARG:HG3	1:A:250:TYR:CZ	2.46	0.51
3:J:388:ILE:HD13	3:J:449:ALA:CB	2.39	0.51
1:A:241:THR:O	1:A:242:VAL:HG23	2.11	0.51
2:I:37:VAL:HB	2:I:66:TYR:CE1	2.46	0.51
3:D:99:ASN:HD21	3:D:103:LEU:HD11	1.76	0.51
3:D:224:PRO:O	3:D:336:ARG:NH1	2.44	0.51
3:M:383:GLU:HB3	3:M:384:PRO:HD3	1.93	0.51
3:J:383:GLU:HB3	3:J:384:PRO:HD3	1.93	0.51
3:J:231:VAL:O	3:J:235:VAL:HG23	2.11	0.51
1:H:36:LEU:C	1:H:36:LEU:HD23	2.31	0.50
3:G:408:LEU:HD11	3:G:530:VAL:CG2	2.41	0.50
3:D:415:VAL:HG13	3:D:418:VAL:CG2	2.41	0.50
1:K:203:PHE:CZ	1:K:208:LEU:HD13	2.47	0.50
1:H:190:SER:CB	1:H:191:PRO:CD	2.89	0.50
2:F:37:VAL:HB	2:F:66:TYR:CE1	2.46	0.50
3:G:48:GLU:O	3:G:52:THR:HG23	2.12	0.50
3:G:224:PRO:O	3:G:336:ARG:NH1	2.44	0.50
3:M:108:ASP:OD1	3:M:466:LYS:NZ	2.44	0.50
3:D:415:VAL:HG13	3:D:415:VAL:O	2.11	0.50
1:H:182:MET:HE2	1:H:254:VAL:CB	2.40	0.50
3:M:293:VAL:HG22	3:M:294:GLU:H	1.76	0.50
1:H:11:LEU:HD13	1:H:94:LEU:HD12	1.94	0.50
3:G:159:LYS:CE	3:G:284:LEU:HD12	2.42	0.50
1:A:8:LEU:HD23	1:A:95:GLY:HA3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:LEU:C	1:K:36:LEU:HD23	2.33	0.49
3:J:303:PRO:O	3:J:337:ARG:NH1	2.45	0.49
3:D:32:GLN:HE22	3:D:107:ASP:H	1.60	0.49
2:I:2:GLN:NE2	2:I:85:VAL:HG11	2.27	0.49
1:A:221:THR:HG22	1:A:238:SER:OG	2.12	0.49
1:A:11:LEU:CD1	1:A:94:LEU:CD1	2.77	0.49
3:G:397:GLN:O	3:G:398:LEU:HD23	2.12	0.49
3:M:540:THR:H	3:M:543:GLN:HE21	1.60	0.49
3:M:303:PRO:O	3:M:337:ARG:NH1	2.45	0.49
1:H:182:MET:HE1	1:H:254:VAL:HG21	1.93	0.49
3:G:383:GLU:HB3	3:G:384:PRO:HD3	1.94	0.49
3:J:36:PHE:O	3:J:40:VAL:HG23	2.12	0.49
3:J:159:LYS:HE2	3:J:284:LEU:HD12	1.95	0.49
3:D:303:PRO:O	3:D:337:ARG:NH1	2.46	0.49
1:A:59:TRP:NE1	3:D:463:LEU:HD13	2.28	0.49
1:H:167:LEU:HD23	1:H:174:LEU:CD1	2.42	0.49
1:E:208:LEU:HD23	1:E:208:LEU:C	2.33	0.48
3:J:135:LEU:HD21	3:J:162:LYS:HB2	1.95	0.48
3:D:383:GLU:HB3	3:D:384:PRO:HD3	1.94	0.48
1:H:57:VAL:HG11	3:J:111:ASN:CB	2.42	0.48
1:E:203:PHE:CE2	1:E:208:LEU:HD13	2.48	0.48
3:J:71:GLY:O	3:J:72:ASP:C	2.51	0.48
2:I:83:ASN:HD22	2:I:84:HIS:N	2.08	0.48
1:H:214:ARG:HG3	1:H:250:TYR:CZ	2.49	0.48
3:J:32:GLN:HE22	3:J:107:ASP:H	1.62	0.48
3:G:112:LEU:HD21	3:G:144:ARG:NH1	2.28	0.48
3:M:71:GLY:O	3:M:72:ASP:C	2.52	0.48
1:K:57:VAL:HG12	1:K:58:SER:N	2.28	0.48
1:K:203:PHE:CE2	1:K:208:LEU:HD13	2.48	0.48
3:J:21:ALA:HB1	3:J:139:LEU:HD21	1.95	0.48
1:H:197:THR:HG21	2:I:99:MET:HG2	1.96	0.48
1:E:214:ARG:NH1	1:E:215:ASN:HD22	2.11	0.48
3:G:303:PRO:O	3:G:337:ARG:NH1	2.46	0.48
1:K:44:GLU:OE1	3:M:469:VAL:HG22	2.14	0.48
1:H:214:ARG:NH1	1:H:215:ASN:HD22	2.12	0.48
1:E:214:ARG:HG3	1:E:250:TYR:CZ	2.49	0.48
1:K:241:THR:O	1:K:242:VAL:HG23	2.14	0.48
3:D:216:VAL:CG2	3:D:235:VAL:HG21	2.44	0.48
3:G:518:GLU:OE1	3:G:518:GLU:HA	2.14	0.48
3:M:494:ASP:OD1	3:M:496:THR:HB	2.14	0.48
1:H:57:VAL:HG11	3:J:111:ASN:CG	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:71:GLY:O	3:D:72:ASP:C	2.51	0.47
1:A:208:LEU:HD23	1:A:208:LEU:C	2.35	0.47
3:J:85:GLY:O	3:J:87:MET:N	2.47	0.47
1:K:57:VAL:HG11	3:M:111:ASN:CG	2.34	0.47
1:H:182:MET:HE1	1:H:254:VAL:CG2	2.43	0.47
3:G:71:GLY:O	3:G:72:ASP:C	2.52	0.47
3:M:518:GLU:OE1	3:M:518:GLU:HA	2.13	0.47
3:J:415:VAL:HG13	3:J:418:VAL:CG2	2.43	0.47
3:D:99:ASN:ND2	3:D:103:LEU:HD11	2.28	0.47
3:J:31:LEU:HG	3:J:74:LEU:HD22	1.96	0.47
3:M:34:CYS:HB3	3:M:39:HIS:NE2	2.30	0.47
1:H:78:ALA:HB1	1:H:137:ILE:CD1	2.44	0.47
1:H:182:MET:CE	1:H:254:VAL:CB	2.92	0.47
3:M:85:GLY:O	3:M:87:MET:N	2.47	0.47
1:K:8:LEU:HD23	1:K:95:GLY:HA3	1.95	0.47
1:K:44:GLU:OE2	3:M:469:VAL:HG22	2.15	0.47
1:E:254:VAL:CG1	1:E:263:LEU:HB3	2.45	0.47
1:H:77:GLU:HG2	1:H:140:ARG:NH1	2.30	0.47
1:H:254:VAL:HG13	1:H:254:VAL:O	2.14	0.47
1:E:203:PHE:CZ	1:E:208:LEU:HD13	2.50	0.47
3:J:494:ASP:OD1	3:J:496:THR:HB	2.15	0.47
1:E:99:GLY:N	1:E:103:THR:O	2.44	0.47
3:G:293:VAL:HG22	3:G:294:GLU:H	1.80	0.47
3:J:214:TRP:CD1	3:J:343:VAL:HG11	2.49	0.47
3:D:194:ALA:HB1	3:D:455:VAL:CG1	2.44	0.47
1:H:80:LYS:HD2	1:H:140:ARG:HH12	1.80	0.47
3:D:518:GLU:HA	3:D:518:GLU:OE1	2.15	0.47
3:D:48:GLU:O	3:D:52:THR:HG23	2.15	0.47
3:G:194:ALA:HB1	3:G:455:VAL:HG13	1.97	0.47
3:J:513:ILE:HG22	3:J:516:LEU:HD11	1.97	0.46
3:D:34:CYS:HB3	3:D:39:HIS:NE2	2.31	0.46
3:M:223:PHE:N	3:M:224:PRO:CD	2.79	0.46
3:J:518:GLU:HA	3:J:518:GLU:OE1	2.14	0.46
3:J:223:PHE:N	3:J:224:PRO:CD	2.79	0.46
1:K:53:TRP:CZ3	3:M:527:THR:HG22	2.51	0.46
1:K:93:LEU:C	1:K:94:LEU:HD23	2.36	0.46
3:G:85:GLY:O	3:G:87:MET:N	2.48	0.46
3:G:472:ARG:NH2	3:G:492:GLU:O	2.49	0.46
2:B:2:GLN:NE2	2:B:85:VAL:HG11	2.31	0.46
3:D:42:LEU:O	3:D:46:VAL:HG23	2.16	0.46
1:K:99:GLY:O	1:K:100:PRO:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:572:GLY:O	3:G:576:VAL:HG23	2.15	0.45
1:H:17:PRO:HB2	1:H:21:THR:HG22	1.99	0.45
3:J:541:LYS:HZ2	3:J:545:LYS:HE3	1.82	0.45
1:E:221:THR:HG22	1:E:238:SER:OG	2.16	0.45
3:D:422:THR:O	3:D:426:VAL:HG23	2.16	0.45
3:G:494:ASP:OD1	3:G:496:THR:HB	2.16	0.45
1:E:93:LEU:HA	1:E:93:LEU:HD12	1.73	0.45
1:A:187:ARG:NH1	2:B:96:ASP:OD1	2.49	0.45
3:G:33:GLN:HE21	3:G:112:LEU:HD13	1.76	0.45
2:F:34:ASP:O	2:F:84:HIS:HD2	2.00	0.45
3:D:73:LYS:O	3:D:76:THR:HB	2.17	0.45
3:M:185:LEU:HD12	3:M:185:LEU:HA	1.61	0.45
1:A:56:GLN:NE2	1:A:57:VAL:H	2.15	0.45
1:H:242:VAL:HG22	1:H:250:TYR:CZ	2.51	0.45
1:H:112:LEU:HD12	1:H:113:ASN:H	1.82	0.45
3:G:223:PHE:N	3:G:224:PRO:CD	2.79	0.45
1:E:42:ARG:NH1	3:G:498:VAL:O	2.50	0.45
3:D:194:ALA:HB1	3:D:455:VAL:HG13	1.99	0.45
1:E:59:TRP:NE1	3:G:463:LEU:HD13	2.32	0.45
1:A:56:GLN:HE21	1:A:57:VAL:H	1.64	0.44
3:D:99:ASN:O	3:D:103:LEU:HD12	2.16	0.44
3:D:223:PHE:N	3:D:224:PRO:CD	2.79	0.44
1:H:99:GLY:O	1:H:100:PRO:C	2.56	0.44
3:M:112:LEU:O	3:M:113:PRO:C	2.55	0.44
1:K:57:VAL:CG1	1:K:58:SER:N	2.80	0.44
1:E:57:VAL:CG1	1:E:58:SER:N	2.80	0.44
3:G:349:LEU:HD22	3:G:377:PHE:CG	2.52	0.44
3:D:85:GLY:O	3:D:87:MET:N	2.50	0.44
1:A:99:GLY:O	1:A:100:PRO:C	2.55	0.44
3:J:281:LYS:HB3	3:J:282:PRO:HD2	2.00	0.44
1:H:11:LEU:N	1:H:11:LEU:HD12	2.30	0.44
1:H:57:VAL:HG12	1:H:58:SER:N	2.33	0.44
1:H:190:SER:CB	1:H:191:PRO:HD2	2.48	0.44
3:M:32:GLN:HE22	3:M:107:ASP:H	1.66	0.44
3:D:54:VAL:HG12	2:F:88:SER:HB3	1.99	0.44
1:H:254:VAL:CG1	1:H:263:LEU:HB3	2.48	0.44
3:M:415:VAL:HG13	3:M:418:VAL:HG23	1.99	0.44
1:K:99:GLY:N	1:K:103:THR:O	2.42	0.44
1:E:112:LEU:HD12	1:E:113:ASN:H	1.82	0.44
3:M:151:ALA:HB2	3:M:250:LEU:HD22	1.99	0.44
3:J:415:VAL:HG12	3:J:415:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:GLY:O	1:E:100:PRO:C	2.55	0.44
2:B:37:VAL:HB	2:B:66:TYR:CE1	2.52	0.44
3:D:112:LEU:O	3:D:113:PRO:C	2.56	0.44
3:J:112:LEU:O	3:J:113:PRO:C	2.56	0.44
3:G:32:GLN:HE22	3:G:107:ASP:H	1.65	0.44
3:G:34:CYS:HB3	3:G:39:HIS:NE2	2.33	0.44
1:H:241:THR:O	1:H:242:VAL:HG23	2.18	0.44
3:J:349:LEU:HD22	3:J:377:PHE:CG	2.53	0.44
3:D:551:PHE:O	3:D:554:PHE:HB3	2.18	0.44
1:K:214:ARG:HB2	1:K:250:TYR:CE2	2.52	0.43
1:A:42:ARG:NH1	3:D:498:VAL:O	2.52	0.43
3:D:135:LEU:HD21	3:D:162:LYS:HB2	1.99	0.43
3:M:347:LEU:CB	3:M:482:VAL:HG21	2.48	0.43
3:G:551:PHE:O	3:G:554:PHE:HB3	2.18	0.43
1:E:106:PRO:HG3	1:E:122:LEU:HD22	2.00	0.43
2:F:7:ILE:HD13	2:F:82:VAL:CG2	2.49	0.43
1:E:68:LEU:HA	1:E:68:LEU:HD23	1.81	0.43
1:K:197:THR:HG21	2:L:99:MET:HG2	2.00	0.43
3:M:551:PHE:O	3:M:554:PHE:HB3	2.19	0.43
3:M:472:ARG:NH2	3:M:492:GLU:O	2.52	0.43
1:H:99:GLY:N	1:H:103:THR:O	2.42	0.43
1:K:83:GLY:O	1:K:84:GLY:O	2.37	0.43
1:A:26:VAL:HG21	1:A:68:LEU:HD13	1.99	0.43
1:H:203:PHE:CE2	1:H:208:LEU:HD13	2.53	0.43
1:A:94:LEU:HD12	1:A:94:LEU:N	2.33	0.43
3:G:112:LEU:O	3:G:113:PRO:C	2.57	0.43
1:A:214:ARG:HB2	1:A:250:TYR:CE2	2.54	0.43
3:D:44:ASN:O	3:D:48:GLU:HG3	2.19	0.43
3:M:133:THR:O	3:M:136:LYS:N	2.52	0.43
3:D:212:LYS:O	3:D:216:VAL:HG23	2.18	0.43
3:D:133:THR:O	3:D:136:LYS:N	2.52	0.43
1:H:42:ARG:NH1	3:J:498:VAL:O	2.52	0.43
1:A:44:GLU:CD	3:D:469:VAL:HG22	2.39	0.43
1:A:203:PHE:CE2	1:A:208:LEU:HD13	2.54	0.43
1:H:126:THR:HA	1:H:142:GLN:HE22	1.84	0.43
1:H:56:GLN:NE2	1:H:57:VAL:H	2.17	0.42
1:E:59:TRP:CD1	3:G:463:LEU:HD13	2.54	0.42
1:E:83:GLY:O	1:E:84:GLY:O	2.36	0.42
1:K:78:ALA:HB1	1:K:137:ILE:HD13	2.01	0.42
3:J:397:GLN:O	3:J:398:LEU:HD23	2.19	0.42
3:M:281:LYS:HB3	3:M:282:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LEU:C	2:B:40:LEU:HD23	2.40	0.42
3:G:415:VAL:O	3:G:415:VAL:CG1	2.68	0.42
3:G:97:GLU:HA	3:G:100:GLU:HG3	2.01	0.42
3:D:526:GLN:O	3:D:530:VAL:HG23	2.19	0.42
3:J:572:GLY:O	3:J:576:VAL:HG23	2.19	0.42
3:D:172:ALA:HB2	3:J:293:VAL:O	2.18	0.42
1:E:122:LEU:HD12	1:E:122:LEU:H	1.84	0.42
3:J:497:TYR:O	3:J:499:PRO:HD3	2.20	0.42
3:D:281:LYS:HB3	3:D:282:PRO:HD2	2.00	0.42
3:G:231:VAL:O	3:G:235:VAL:HG23	2.20	0.42
3:M:326:PHE:HA	3:M:329:MET:HE2	2.01	0.42
1:E:53:TRP:CZ3	3:G:527:THR:HG22	2.54	0.42
3:G:21:ALA:HB1	3:G:139:LEU:HD21	2.02	0.42
3:M:214:TRP:CD1	3:M:343:VAL:HG11	2.54	0.42
3:G:317:LYS:O	3:G:321:GLU:HG2	2.20	0.42
3:J:551:PHE:O	3:J:554:PHE:HB3	2.20	0.42
1:E:167:LEU:HD23	1:E:174:LEU:CD1	2.49	0.42
3:M:33:GLN:HE21	3:M:112:LEU:HG	1.83	0.42
1:H:56:GLN:HE21	1:H:57:VAL:H	1.67	0.42
3:M:497:TYR:O	3:M:499:PRO:HD3	2.20	0.42
1:E:11:LEU:HD12	1:E:11:LEU:N	2.34	0.42
3:G:216:VAL:CG2	3:G:235:VAL:HG21	2.50	0.42
3:G:472:ARG:CZ	3:G:491:LEU:HD22	2.49	0.42
3:M:133:THR:O	3:M:134:PHE:C	2.58	0.42
3:G:525:LYS:O	3:G:548:MET:HE1	2.19	0.42
2:F:24:ASN:HB3	2:F:65:LEU:HD11	2.00	0.42
1:E:59:TRP:CE3	1:E:62:GLU:HG3	2.55	0.42
3:M:97:GLU:HA	3:M:100:GLU:HG3	2.01	0.42
3:G:430:LEU:HD22	3:G:453:LEU:HD23	2.01	0.41
3:J:34:CYS:HB3	3:J:39:HIS:NE2	2.35	0.41
1:K:11:LEU:CD2	1:K:71:LYS:HG2	2.50	0.41
3:D:89:ASP:O	3:D:92:ALA:HB3	2.19	0.41
3:D:412:THR:OG1	3:D:423:LEU:HD13	2.20	0.41
3:M:575:LEU:HD12	3:M:575:LEU:O	2.21	0.41
3:M:532:LEU:HD13	3:M:547:VAL:HG11	2.02	0.41
3:J:525:LYS:O	3:J:548:MET:HE1	2.20	0.41
3:D:317:LYS:O	3:D:321:GLU:HG2	2.21	0.41
1:A:44:GLU:OE2	3:D:469:VAL:HG22	2.20	0.41
3:J:347:LEU:CB	3:J:482:VAL:HG21	2.49	0.41
3:G:497:TYR:O	3:G:499:PRO:HD3	2.21	0.41
3:G:290:ILE:HD13	3:G:290:ILE:HG21	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:HB1	1:A:137:ILE:HD13	2.02	0.41
1:H:59:TRP:CE3	1:H:62:GLU:HG3	2.54	0.41
1:A:44:GLU:HG3	3:D:417:GLN:HE21	1.83	0.41
3:G:194:ALA:HB1	3:G:455:VAL:HG11	2.01	0.41
1:K:59:TRP:CE3	1:K:62:GLU:HG3	2.54	0.41
3:J:133:THR:O	3:J:136:LYS:N	2.53	0.41
3:M:119:GLU:O	3:M:122:VAL:HG13	2.20	0.41
3:M:415:VAL:HG12	3:M:415:VAL:O	2.19	0.41
3:G:388:ILE:HD13	3:G:449:ALA:HB2	2.02	0.41
3:D:494:ASP:OD1	3:D:496:THR:HB	2.21	0.41
3:D:497:TYR:O	3:D:499:PRO:HD3	2.21	0.41
3:M:349:LEU:HD22	3:M:377:PHE:CG	2.56	0.41
1:K:126:THR:HA	1:K:142:GLN:HE22	1.85	0.41
3:D:97:GLU:HA	3:D:100:GLU:HG3	2.02	0.41
3:J:415:VAL:HG13	3:J:415:VAL:O	2.21	0.41
2:F:27:VAL:HG21	2:F:37:VAL:HG21	2.01	0.41
3:J:408:LEU:HD11	3:J:530:VAL:CG2	2.51	0.41
1:K:5:LEU:HA	1:K:5:LEU:HD23	1.92	0.41
3:J:42:LEU:HD22	3:J:73:LYS:HG3	2.01	0.41
3:J:388:ILE:HD13	3:J:449:ALA:HB2	2.02	0.41
3:D:71:GLY:HA3	3:D:98:ARG:NH1	2.36	0.41
3:G:293:VAL:HG22	3:G:294:GLU:N	2.36	0.41
3:J:112:LEU:HA	3:J:112:LEU:HD12	1.84	0.41
2:B:84:HIS:O	2:B:85:VAL:C	2.59	0.41
1:H:21:THR:HG23	1:H:22:PRO:HD2	2.03	0.41
1:E:78:ALA:HB1	1:E:137:ILE:CD1	2.51	0.41
3:M:71:GLY:HA3	3:M:98:ARG:NH1	2.36	0.41
3:M:217:ALA:HB3	3:M:343:VAL:HG13	2.03	0.41
1:A:83:GLY:O	1:A:84:GLY:O	2.38	0.41
3:M:25:ILE:O	3:M:26:ALA:C	2.58	0.40
1:A:44:GLU:OE2	3:D:417:GLN:HG3	2.21	0.40
3:J:343:VAL:O	3:J:344:VAL:C	2.60	0.40
3:D:99:ASN:ND2	3:D:103:LEU:CD1	2.84	0.40
1:A:59:TRP:CE3	1:A:62:GLU:HG3	2.56	0.40
3:G:518:GLU:O	3:G:519:LYS:C	2.60	0.40
1:E:8:LEU:HD23	1:E:95:GLY:HA3	2.04	0.40
3:G:133:THR:O	3:G:136:LYS:N	2.54	0.40
3:J:472:ARG:NH1	3:J:491:LEU:HD22	2.37	0.40
3:J:541:LYS:NZ	3:J:545:LYS:CE	2.84	0.40
3:D:518:GLU:O	3:D:519:LYS:C	2.59	0.40
3:G:412:THR:OG1	3:G:423:LEU:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:HG2	1:A:122:LEU:HD13	2.03	0.40
3:J:541:LYS:HZ3	3:J:545:LYS:HE3	1.83	0.40
1:A:126:THR:HA	1:A:142:GLN:HE22	1.86	0.40
2:L:89:GLN:O	2:L:90:PRO:C	2.60	0.40
3:J:97:GLU:HA	3:J:100:GLU:HG3	2.02	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	262/271 (97%)	238 (91%)	19 (7%)	5 (2%)	10	41
1	E	262/271 (97%)	235 (90%)	22 (8%)	5 (2%)	10	41
1	H	262/271 (97%)	235 (90%)	21 (8%)	6 (2%)	8	35
1	K	262/271 (97%)	235 (90%)	22 (8%)	5 (2%)	10	41
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	F	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	I	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	L	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
3	D	581/585 (99%)	534 (92%)	42 (7%)	5 (1%)	21	62
3	G	581/585 (99%)	539 (93%)	37 (6%)	5 (1%)	21	62
3	J	581/585 (99%)	536 (92%)	40 (7%)	5 (1%)	21	62
3	M	581/585 (99%)	541 (93%)	35 (6%)	5 (1%)	21	62
All	All	3760/3820 (98%)	3456 (92%)	263 (7%)	41 (1%)	17	56

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASP
1	A	191	PRO
3	D	80	LEU
3	D	129	ASP
3	D	442	GLU
1	E	145	ASP
1	E	191	PRO
3	G	80	LEU
3	G	129	ASP
3	G	442	GLU
1	H	145	ASP
1	H	190	SER
1	H	191	PRO
3	J	80	LEU
3	J	129	ASP
3	J	442	GLU
1	K	145	ASP
1	K	191	PRO
3	M	80	LEU
3	M	129	ASP
3	M	442	GLU
1	A	84	GLY
1	E	84	GLY
1	H	84	GLY
1	K	84	GLY
1	A	100	PRO
3	D	113	PRO
1	E	100	PRO
1	H	100	PRO
1	K	100	PRO
3	M	86	GLU
3	D	86	GLU
3	G	86	GLU
3	J	86	GLU
3	J	113	PRO
3	M	113	PRO
1	A	190	SER
1	E	190	SER
3	G	113	PRO
1	K	190	SER
1	H	228	PRO

5.3.2 Protein sidechains ⓘ

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/224 (97%)	203 (93%)	15 (7%)	19	54
1	E	218/224 (97%)	202 (93%)	16 (7%)	17	51
1	H	218/224 (97%)	202 (93%)	16 (7%)	17	51
1	K	218/224 (97%)	203 (93%)	15 (7%)	19	54
2	B	94/94 (100%)	87 (93%)	7 (7%)	17	50
2	F	94/94 (100%)	84 (89%)	10 (11%)	8	30
2	I	94/94 (100%)	88 (94%)	6 (6%)	22	58
2	L	94/94 (100%)	87 (93%)	7 (7%)	17	50
3	D	510/511 (100%)	478 (94%)	32 (6%)	22	58
3	G	510/511 (100%)	477 (94%)	33 (6%)	21	56
3	J	510/511 (100%)	476 (93%)	34 (7%)	20	55
3	M	510/511 (100%)	478 (94%)	32 (6%)	22	58
All	All	3288/3316 (99%)	3065 (93%)	223 (7%)	20	55

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	27	SER
1	A	36	LEU
1	A	116	GLU
1	A	140	ARG
1	A	177	LYS
1	A	190	SER
1	A	194	SER
1	A	214	ARG
1	A	221	THR
1	A	237	SER
1	A	242	VAL
1	A	244	SER
1	A	255	GLN

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Mol	Chain	Res	Type
1	A	261	GLN
2	B	1	ILE
2	B	33	SER
2	B	45	ARG
2	B	70	PHE
2	B	74	GLU
2	B	83	ASN
2	B	94	LYS
3	D	3	HIS
3	D	6	GLU
3	D	34	CYS
3	D	60	GLU
3	D	63	ASP
3	D	76	THR
3	D	79	THR
3	D	98	ARG
3	D	100	GLU
3	D	139	LEU
3	D	193	SER
3	D	222	ARG
3	D	245	CYS
3	D	253	CYS
3	D	257	ARG
3	D	268	GLN
3	D	283	LEU
3	D	292	GLU
3	D	293	VAL
3	D	334	TYR
3	D	337	ARG
3	D	390	GLN
3	D	396	GLU
3	D	433	VAL
3	D	435	SER
3	D	455	VAL
3	D	469	VAL
3	D	484	ARG
3	D	543	GLN
3	D	564	LYS
3	D	565	GLU
3	D	585	LEU
1	E	5	LEU
1	E	10	HIS

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Mol	Chain	Res	Type
1	E	27	SER
1	E	36	LEU
1	E	44	GLU
1	E	116	GLU
1	E	117	PHE
1	E	140	ARG
1	E	190	SER
1	E	194	SER
1	E	214	ARG
1	E	221	THR
1	E	237	SER
1	E	242	VAL
1	E	244	SER
1	E	261	GLN
2	F	1	ILE
2	F	9	VAL
2	F	33	SER
2	F	44	GLU
2	F	47	GLU
2	F	70	PHE
2	F	74	GLU
2	F	83	ASN
2	F	89	GLN
2	F	94	LYS
3	G	3	HIS
3	G	6	GLU
3	G	7	VAL
3	G	34	CYS
3	G	60	GLU
3	G	63	ASP
3	G	79	THR
3	G	98	ARG
3	G	100	GLU
3	G	139	LEU
3	G	193	SER
3	G	204	GLN
3	G	222	ARG
3	G	245	CYS
3	G	253	CYS
3	G	257	ARG
3	G	268	GLN
3	G	334	TYR

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Mol	Chain	Res	Type
3	G	337	ARG
3	G	390	GLN
3	G	396	GLU
3	G	415	VAL
3	G	417	GLN
3	G	424	VAL
3	G	433	VAL
3	G	435	SER
3	G	469	VAL
3	G	478	THR
3	G	484	ARG
3	G	543	GLN
3	G	564	LYS
3	G	565	GLU
3	G	585	LEU
1	H	5	LEU
1	H	10	HIS
1	H	21	THR
1	H	27	SER
1	H	36	LEU
1	H	44	GLU
1	H	116	GLU
1	H	117	PHE
1	H	140	ARG
1	H	194	SER
1	H	214	ARG
1	H	221	THR
1	H	241	THR
1	H	242	VAL
1	H	244	SER
1	H	261	GLN
2	I	1	ILE
2	I	33	SER
2	I	70	PHE
2	I	74	GLU
2	I	83	ASN
2	I	94	LYS
3	J	3	HIS
3	J	6	GLU
3	J	34	CYS
3	J	60	GLU
3	J	63	ASP

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Mol	Chain	Res	Type
3	J	79	THR
3	J	98	ARG
3	J	100	GLU
3	J	139	LEU
3	J	193	SER
3	J	204	GLN
3	J	222	ARG
3	J	245	CYS
3	J	253	CYS
3	J	257	ARG
3	J	268	GLN
3	J	283	LEU
3	J	285	GLU
3	J	292	GLU
3	J	293	VAL
3	J	334	TYR
3	J	337	ARG
3	J	390	GLN
3	J	396	GLU
3	J	415	VAL
3	J	433	VAL
3	J	435	SER
3	J	469	VAL
3	J	482	VAL
3	J	484	ARG
3	J	543	GLN
3	J	564	LYS
3	J	565	GLU
3	J	585	LEU
1	K	10	HIS
1	K	27	SER
1	K	36	LEU
1	K	116	GLU
1	K	117	PHE
1	K	140	ARG
1	K	177	LYS
1	K	190	SER
1	K	194	SER
1	K	214	ARG
1	K	221	THR
1	K	237	SER
1	K	242	VAL

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Mol	Chain	Res	Type
1	K	244	SER
1	K	261	GLN
2	L	1	ILE
2	L	33	SER
2	L	70	PHE
2	L	74	GLU
2	L	83	ASN
2	L	89	GLN
2	L	94	LYS
3	M	3	HIS
3	M	6	GLU
3	M	60	GLU
3	M	79	THR
3	M	98	ARG
3	M	100	GLU
3	M	112	LEU
3	M	139	LEU
3	M	193	SER
3	M	204	GLN
3	M	222	ARG
3	M	245	CYS
3	M	253	CYS
3	M	257	ARG
3	M	268	GLN
3	M	285	GLU
3	M	293	VAL
3	M	334	TYR
3	M	337	ARG
3	M	390	GLN
3	M	396	GLU
3	M	415	VAL
3	M	417	GLN
3	M	433	VAL
3	M	435	SER
3	M	446	MET
3	M	469	VAL
3	M	482	VAL
3	M	484	ARG
3	M	543	GLN
3	M	564	LYS
3	M	565	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	56	GLN
1	A	215	ASN
1	A	255	GLN
1	A	261	GLN
2	B	83	ASN
3	D	33	GLN
3	D	99	ASN
3	D	146	HIS
3	D	535	HIS
3	D	543	GLN
1	E	4	HIS
1	E	56	GLN
1	E	215	ASN
1	E	261	GLN
2	F	83	ASN
3	G	33	GLN
3	G	94	GLN
3	G	535	HIS
3	G	543	GLN
1	H	33	GLN
1	H	56	GLN
1	H	144	GLN
1	H	215	ASN
1	H	261	GLN
2	I	2	GLN
2	I	83	ASN
3	J	33	GLN
3	J	535	HIS
3	J	543	GLN
1	K	33	GLN
1	K	56	GLN
1	K	261	GLN
2	L	83	ASN
3	M	33	GLN
3	M	170	GLN
3	M	535	HIS
3	M	543	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

There are no ligands in this entry.

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, 95th 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	264/271 (97%)	-0.47	0 100 100	12, 27, 64, 98	0
1	E	264/271 (97%)	-0.46	0 100 100	12, 28, 63, 87	0
1	H	264/271 (97%)	-0.34	2 (0%) 87 67	15, 34, 70, 104	0
1	K	264/271 (97%)	-0.42	1 (0%) 93 79	13, 31, 70, 95	0
2	B	99/99 (100%)	-0.47	0 100 100	15, 31, 57, 71	0
2	F	99/99 (100%)	-0.39	0 100 100	16, 38, 70, 92	0
2	I	99/99 (100%)	-0.12	1 (1%) 84 60	18, 51, 83, 98	0
2	L	99/99 (100%)	-0.15	0 100 100	16, 49, 79, 96	0
3	D	583/585 (99%)	-0.44	0 100 100	10, 35, 69, 97	0
3	G	583/585 (99%)	-0.45	2 (0%) 94 84	14, 34, 71, 97	0
3	J	583/585 (99%)	-0.43	1 (0%) 95 87	14, 38, 75, 112	0
3	M	583/585 (99%)	-0.41	2 (0%) 94 84	11, 35, 77, 105	0
All	All	3784/3820 (99%)	-0.41	9 (0%) 95 87	10, 34, 73, 112	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	60	GLU	2.9
3	M	116	VAL	2.7
1	K	102	ASN	2.7
3	M	60	GLU	2.6
2	I	73	THR	2.4
1	H	187	ARG	2.2
3	G	78	ALA	2.2
1	H	101	ASP	2.1
3	G	562	ASP	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.