Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:06 PM GMT

PDB ID	:	4KKA
Title	:	Structure of the E148A mutant of CLC-ec1 deltaNC construct in 100mM fluoride and 20mM Bromide
Authors	:	Lim, H.-H.; Miller, C.
Deposited on	:	2013-05-05
Resolution	:	3.00 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:

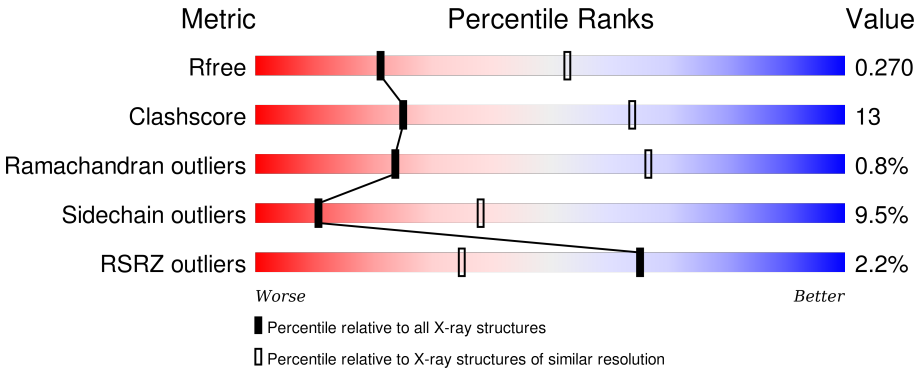
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=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	446	69% 26%
1	B	446	67% 27%
2	C	222	3% 69% 27%
2	E	222	73% 24%
3	D	211	64% 30% 6%

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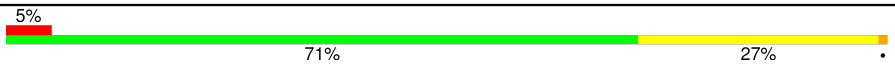
Mol	Chain	Length	Quality of chain
3	F	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13206 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3320	2183	558	559	20			
1	B	441	Total	C	N	O	S	0	0	0
			3300	2172	553	555	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	EXPRESSION TAG	UNP P37019
A	148	ALA	GLU	ENGINEERED MUTATION	UNP P37019
A	461	LYS	-	EXPRESSION TAG	UNP P37019
B	16	MET	-	EXPRESSION TAG	UNP P37019
B	148	ALA	GLU	ENGINEERED MUTATION	UNP P37019
B	461	LYS	-	EXPRESSION TAG	UNP P37019

- Molecule 2 is a protein called Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab, light chain.

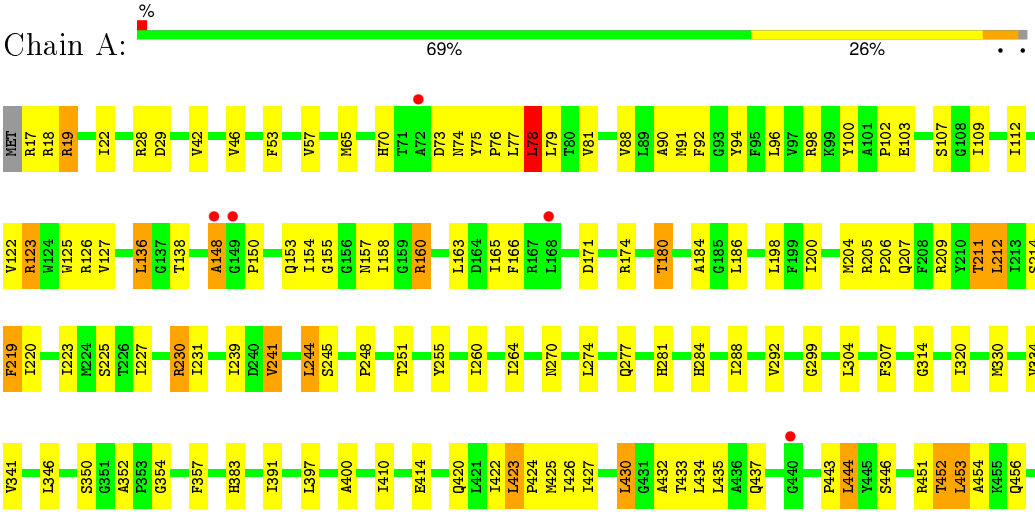
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

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.

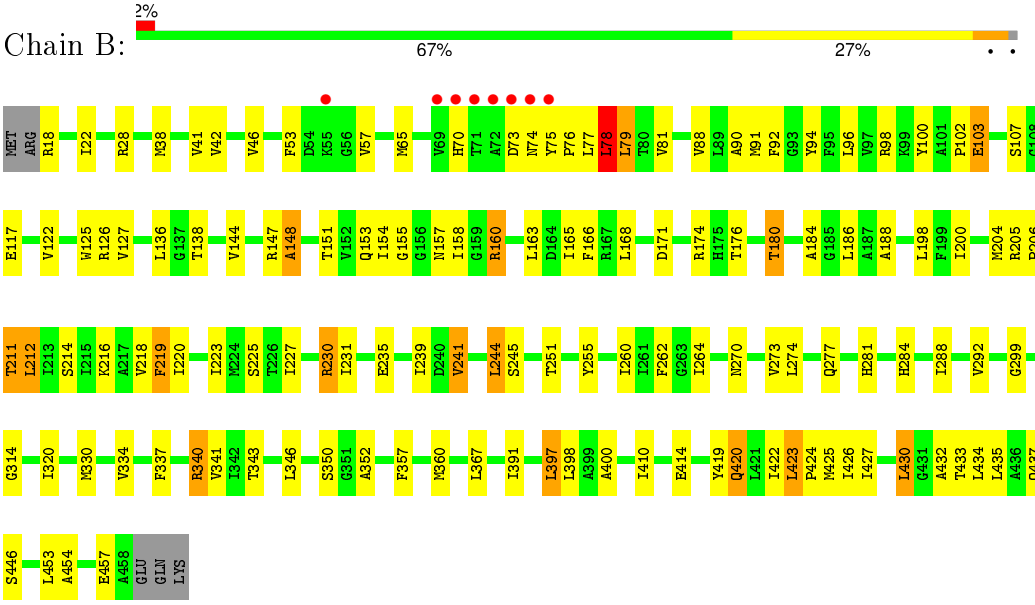
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain A:



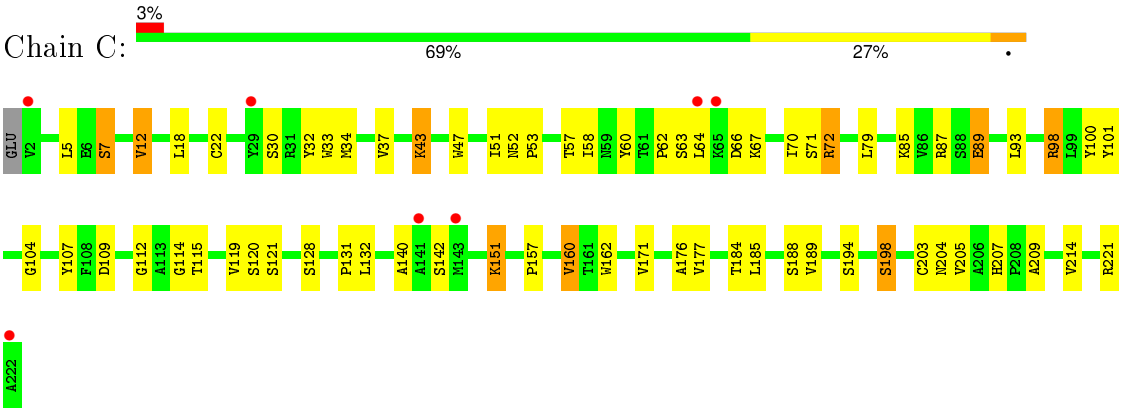
- Molecule 1: H(+)/Cl(-) exchange transporter ClcA

Chain B:



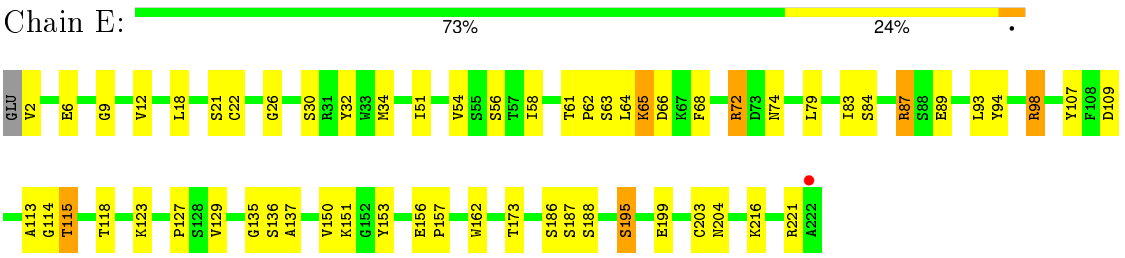
- Molecule 2: Fab, heavy chain

Chain C:



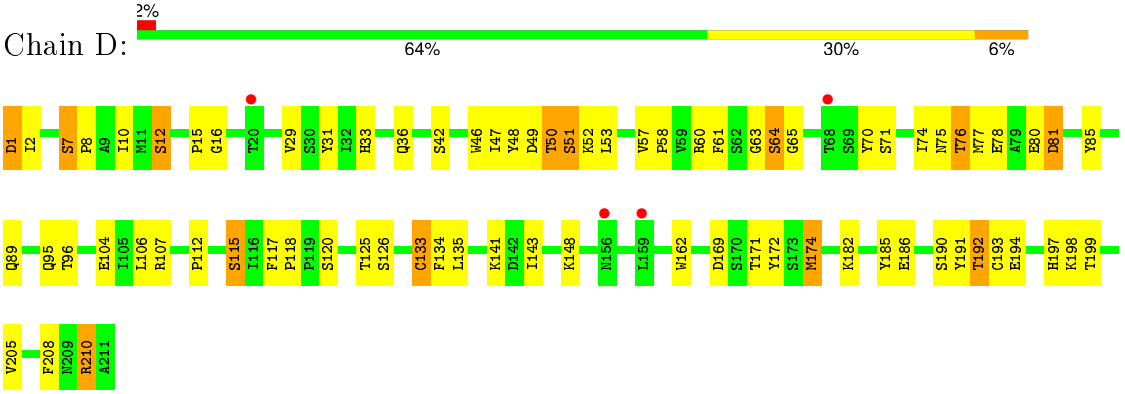
- Molecule 2: Fab, heavy chain

Chain E:



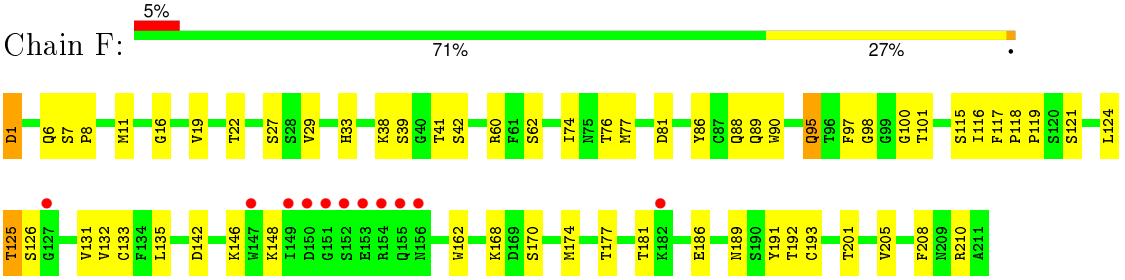
- Molecule 3: Fab, light chain

Chain D:



- Molecule 3: Fab, light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.34Å 99.34Å 170.29Å 90.00° 131.94° 90.00°	Depositor
Resolution (Å)	39.85 – 3.00 39.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.85-3.00) 99.5 (39.85-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.220 , 0.265 0.229 , 0.270	Depositor DCC
R_{free} test set	2818 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.5	EDS
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 57496 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13206	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.43	0/3392	0.58	1/4604 (0.0%)
1	B	0.41	0/3372	0.58	1/4578 (0.0%)
2	C	0.55	0/1721	0.69	0/2355
2	E	0.48	0/1721	0.64	0/2355
3	D	0.46	0/1660	0.64	0/2257
3	F	0.47	0/1660	0.66	0/2257
All	All	0.46	0/13526	0.62	2/18406 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	LEU	CA-CB-CG	6.17	129.50	115.30
1	B	78	LEU	CA-CB-CG	5.93	128.94	115.30

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	3320	0	3475	105	0
1	B	3300	0	3456	109	0
2	C	1672	0	1654	36	0
2	E	1672	0	1654	35	0
3	D	1621	0	1548	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1621	0	1546	42	0
All	All	13206	0	13333	337	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 13.

All (337) 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:19:ARG:HD3	1:B:457:GLU:OE1	1.50	1.11
3:D:95:GLN:N	3:D:95:GLN:OE1	2.03	0.91
3:D:133:CYS:SG	3:D:193:CYS:CB	2.63	0.85
1:B:457:GLU:O	1:B:457:GLU:HG3	1.78	0.81
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.63	0.80
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.15	0.79
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.63	0.79
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.47	0.79
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.64	0.78
3:D:133:CYS:HG	3:D:193:CYS:CB	1.96	0.77
3:D:133:CYS:CB	3:D:193:CYS:HG	1.99	0.75
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.51	0.74
3:F:1:ASP:OD2	3:F:1:ASP:N	2.19	0.74
3:F:132:VAL:HG22	3:F:177:THR:HG23	1.69	0.74
1:A:117:GLU:OE1	1:A:209:ARG:NH1	2.22	0.72
3:F:95:GLN:CD	3:F:95:GLN:H	1.93	0.72
1:A:200:ILE:HA	1:A:204:MET:HB2	1.71	0.71
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.71	0.71
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.25	0.71
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.22	0.71
1:A:219:PHE:HB3	1:B:430:LEU:HD21	1.73	0.71
2:C:176:ALA:HB2	2:C:185:LEU:HD23	1.74	0.70
1:B:422:ILE:HA	1:B:425:MET:HE3	1.73	0.69
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.25	0.69
1:B:200:ILE:HA	1:B:204:MET:HB2	1.75	0.68
1:A:430:LEU:HD21	1:B:219:PHE:HB3	1.76	0.68
1:A:207:GLN:HG2	1:B:28:ARG:NE	2.07	0.67
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.25	0.67
3:F:189:ASN:HA	3:F:210:ARG:HD3	1.74	0.67
1:A:422:ILE:HA	1:A:425:MET:HE3	1.73	0.67
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.75	0.67
3:D:29:VAL:O	3:D:70:TYR:OH	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:49:ASP:O	3:D:51:SER:N	2.26	0.66
3:F:95:GLN:NE2	3:F:95:GLN:H	1.94	0.65
1:B:206:PRO:HG2	1:B:211:THR:HG21	1.78	0.65
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.29	0.65
3:D:133:CYS:CB	3:D:193:CYS:SG	2.83	0.65
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.62	0.65
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.79	0.65
3:D:1:ASP:N	3:D:1:ASP:OD2	2.27	0.64
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.12	0.64
1:A:73:ASP:OD1	1:A:73:ASP:N	2.31	0.64
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.80	0.64
3:D:133:CYS:SG	3:D:193:CYS:HB3	2.38	0.64
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.80	0.64
2:E:129:VAL:HG22	2:E:150:VAL:HG13	1.80	0.64
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.78	0.64
3:F:38:LYS:O	3:F:41:THR:HG22	1.98	0.63
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.80	0.63
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.63	0.63
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.81	0.63
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.34	0.63
3:F:186:GLU:HG2	3:F:210:ARG:HH12	1.64	0.62
1:B:154:ILE:O	1:B:158:ILE:HG12	1.98	0.61
1:B:73:ASP:OD1	1:B:73:ASP:N	2.34	0.61
2:C:160:VAL:HG13	2:C:205:VAL:HG22	1.82	0.61
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.82	0.61
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.83	0.61
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.82	0.60
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.82	0.60
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.37	0.60
2:E:32:TYR:O	2:E:72:ARG:NH2	2.35	0.59
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.37	0.59
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.38	0.59
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.84	0.59
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.85	0.59
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.38	0.58
2:E:12:VAL:HG11	2:E:18:LEU:HD22	1.83	0.58
1:A:198:LEU:HD11	1:B:198:LEU:HD11	1.85	0.58
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.85	0.58
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.86	0.58
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.18	0.58
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.39	0.58
3:F:95:GLN:N	3:F:95:GLN:CD	2.55	0.58
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.39	0.58
1:B:88:VAL:HA	1:B:91:MET:HE2	1.86	0.58
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.20	0.57
2:E:61:THR:O	2:E:63:SER:N	2.37	0.57
2:E:9:GLY:H	2:E:115:THR:HG21	1.68	0.57
3:D:2:ILE:O	3:D:96:THR:HG21	2.05	0.56
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.85	0.56
1:A:18:ARG:HH11	1:B:457:GLU:CB	2.18	0.56
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.88	0.56
1:A:154:ILE:O	1:A:158:ILE:HG12	2.04	0.56
3:D:36:GLN:HB2	3:D:85:TYR:CE2	2.41	0.56
1:A:437:GLN:HE21	1:B:216:LYS:NZ	2.04	0.56
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.88	0.56
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.40	0.55
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.38	0.55
3:F:7:SER:HB3	3:F:22:THR:HB	1.88	0.55
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.88	0.55
1:A:88:VAL:HA	1:A:91:MET:HE2	1.88	0.55
2:E:94:TYR:O	2:E:114:GLY:HA2	2.06	0.55
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.22	0.55
1:A:314:GLY:O	1:A:340:ARG:NH2	2.40	0.55
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.07	0.54
1:A:148:ALA:HB1	1:A:357:PHE:HB3	1.90	0.54
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.89	0.54
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.07	0.54
3:D:169:ASP:OD1	3:D:171:THR:OG1	2.17	0.54
1:A:248:PRO:HB3	2:C:104:GLY:HA3	1.90	0.53
1:B:314:GLY:O	1:B:340:ARG:NH2	2.41	0.53
2:E:173:THR:HG23	2:E:187:SER:HB2	1.90	0.53
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.91	0.53
1:B:214:SER:O	1:B:218:VAL:HG23	2.08	0.53
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.90	0.53
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.90	0.53
1:B:112:ILE:HG13	1:B:153:GLN:HA	1.90	0.53
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.24	0.52
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.91	0.52
2:C:151:LYS:HB3	2:C:184:THR:HG23	1.92	0.52
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.78	0.52
1:A:227:ILE:O	1:A:231:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:O	1:B:231:ILE:HG12	2.10	0.52
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.91	0.52
2:E:129:VAL:O	2:E:216:LYS:HE3	2.09	0.52
1:A:112:ILE:HG13	1:A:153:GLN:HA	1.92	0.51
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.46	0.51
1:B:239:ILE:HD13	1:B:320:ILE:HG21	1.92	0.51
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.92	0.51
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.93	0.51
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.91	0.51
1:B:212:LEU:H	1:B:212:LEU:HD12	1.75	0.51
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.92	0.51
1:A:219:PHE:CE2	1:B:426:ILE:HG23	2.46	0.51
1:A:78:LEU:HD21	1:A:307:PHE:CE1	2.46	0.51
3:D:12:SER:HA	3:D:104:GLU:O	2.10	0.51
1:A:414:GLU:OE1	1:B:419:TYR:OH	2.21	0.50
1:B:42:VAL:O	1:B:46:VAL:HG23	2.12	0.50
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.27	0.50
3:D:46:TRP:O	3:D:57:VAL:HG21	2.11	0.50
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.41	0.50
1:A:214:SER:O	1:A:218:VAL:HG23	2.11	0.50
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.26	0.50
3:D:112:PRO:HG3	3:D:143:ILE:HD11	1.92	0.50
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.47	0.50
1:A:100:TYR:O	1:A:126:ARG:NH1	2.41	0.50
1:A:427:ILE:HD11	1:B:227:ILE:HD11	1.93	0.49
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.47	0.49
3:F:6:GLN:NE2	3:F:100:GLY:H	2.10	0.49
2:C:89:GLU:OE2	2:C:89:GLU:N	2.45	0.49
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.27	0.49
1:A:239:ILE:HD13	1:A:320:ILE:HG21	1.94	0.49
3:D:74:ILE:HD13	3:D:81:ASP:OD2	2.12	0.49
1:A:434:LEU:HD11	1:B:220:ILE:HD11	1.94	0.49
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.27	0.49
3:D:31:TYR:HA	3:D:50:THR:OG1	2.12	0.49
2:E:135:GLY:O	2:E:137:ALA:N	2.39	0.49
1:B:148:ALA:HB1	1:B:357:PHE:HB3	1.94	0.49
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.95	0.49
1:B:78:LEU:HD13	1:B:79:LEU:HD23	1.95	0.49
1:A:219:PHE:HE2	1:B:426:ILE:HG23	1.78	0.48
3:F:186:GLU:HG2	3:F:210:ARG:NH1	2.28	0.48
1:A:274:LEU:O	1:A:277:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HD21	1:B:307:PHE:CE1	2.48	0.48
3:D:182:LYS:HE2	3:D:186:GLU:OE1	2.13	0.48
3:D:15:PRO:HA	3:D:77:MET:O	2.13	0.48
1:A:19:ARG:CD	1:B:457:GLU:OE1	2.42	0.48
1:A:78:LEU:HD13	1:A:79:LEU:HD23	1.95	0.48
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.49	0.48
2:C:131:PRO:O	2:C:132:LEU:HD23	2.14	0.48
2:C:151:LYS:HE3	2:C:151:LYS:HB2	1.61	0.48
1:A:410:ILE:O	1:A:414:GLU:HG3	2.14	0.47
2:C:64:LEU:HD11	2:C:87:ARG:HH12	1.79	0.47
3:D:106:LEU:HD23	3:D:107:ARG:N	2.29	0.47
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.96	0.47
3:D:191:TYR:HB2	3:D:208:PHE:CE2	2.49	0.47
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.77	0.47
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.96	0.47
3:D:53:LEU:HD13	3:D:57:VAL:HG12	1.96	0.47
2:E:113:ALA:HA	3:F:42:SER:OG	2.15	0.47
1:B:98:ARG:HB3	1:B:288:ILE:HG13	1.97	0.47
2:C:64:LEU:HD12	2:C:67:LYS:HD3	1.96	0.47
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.29	0.47
3:F:11:MET:CE	3:F:19:VAL:HG13	2.45	0.47
1:B:100:TYR:O	1:B:126:ARG:NH1	2.44	0.47
3:D:115:SER:HB3	3:D:117:PHE:CE1	2.49	0.47
3:F:191:TYR:HB2	3:F:208:PHE:CE2	2.50	0.47
1:B:430:LEU:HA	1:B:430:LEU:HD12	1.55	0.47
1:B:103:GLU:H	1:B:103:GLU:HG3	1.29	0.47
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.97	0.47
1:B:176:THR:O	1:B:180:THR:HG23	2.15	0.46
3:D:60:ARG:HD2	3:D:76:THR:O	2.15	0.46
2:E:64:LEU:HB3	2:E:65:LYS:H	1.54	0.46
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.97	0.46
3:D:162:TRP:CG	3:D:174:MET:HG3	2.50	0.46
1:A:123:ARG:HH21	1:A:126:ARG:HD3	1.79	0.46
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.50	0.46
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.50	0.46
3:F:118:PRO:HB3	3:F:208:PHE:CE1	2.51	0.46
1:B:274:LEU:O	1:B:277:GLN:HB2	2.15	0.46
2:C:52:ASN:ND2	2:C:57:THR:HB	2.31	0.46
2:C:7:SER:HA	2:C:115:THR:HG21	1.98	0.46
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.98	0.46
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:PHE:HD2	2:E:83:ILE:HG12	1.81	0.46
3:D:197:HIS:ND1	3:D:199:THR:OG1	2.35	0.46
3:D:78:GLU:O	3:D:81:ASP:HB2	2.16	0.46
1:B:53:PHE:O	1:B:57:VAL:HG23	2.16	0.46
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.82	0.46
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.51	0.46
1:A:22:ILE:HD13	1:B:454:ALA:HB2	1.98	0.45
1:B:160:ARG:O	1:B:163:LEU:HB3	2.16	0.45
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.71	0.45
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.97	0.45
3:F:186:GLU:HA	3:F:210:ARG:NH1	2.31	0.45
2:E:221:ARG:NH1	3:F:118:PRO:HD2	2.31	0.45
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.99	0.45
1:B:109:ILE:HG23	1:B:204:MET:SD	2.56	0.45
1:A:330:MET:HE2	1:A:334:VAL:HG23	1.97	0.45
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.81	0.45
1:A:98:ARG:HB3	1:A:288:ILE:HG13	1.99	0.45
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.51	0.45
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.98	0.45
2:C:107:TYR:HB3	3:D:33:HIS:CE1	2.51	0.45
1:B:273:VAL:O	1:B:277:GLN:HG3	2.16	0.45
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.98	0.45
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.51	0.45
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.20	0.45
1:B:241:VAL:HG13	1:B:244:LEU:HD21	1.99	0.45
1:B:91:MET:HG2	1:B:292:VAL:O	2.17	0.45
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.34	0.45
1:A:91:MET:HG2	1:A:292:VAL:O	2.17	0.44
1:B:410:ILE:O	1:B:414:GLU:HG3	2.17	0.44
1:A:18:ARG:O	1:A:22:ILE:HG13	2.16	0.44
3:F:90:TRP:CE3	3:F:95:GLN:HG3	2.52	0.44
1:A:184:ALA:HB1	1:A:225:SER:CB	2.48	0.44
1:A:53:PHE:O	1:A:57:VAL:HG23	2.17	0.44
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.53	0.44
2:C:188:SER:HB3	3:D:134:PHE:CE2	2.51	0.44
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.47	0.44
3:D:89:GLN:O	3:D:95:GLN:HB2	2.17	0.44
3:D:64:SER:OG	3:D:65:GLY:N	2.48	0.44
3:F:6:GLN:HA	3:F:22:THR:O	2.18	0.44
1:B:78:LEU:HD11	1:B:307:PHE:CZ	2.53	0.44
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.51	0.44
1:A:90:ALA:HB2	1:A:299:GLY:HA3	2.00	0.44
1:A:180:THR:HB	1:A:218:VAL:HA	1.99	0.44
1:B:75:TYR:HA	1:B:78:LEU:HD12	1.99	0.44
2:E:87:ARG:HH21	2:E:89:GLU:CB	2.31	0.44
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.98	0.44
1:A:426:ILE:HG23	1:B:219:PHE:HE2	1.83	0.43
2:E:113:ALA:HA	3:F:42:SER:HG	1.83	0.43
3:D:174:MET:HB3	3:D:174:MET:HE2	1.81	0.43
1:B:165:ILE:HG22	1:B:166:PHE:CD2	2.53	0.43
1:A:160:ARG:O	1:A:163:LEU:HB3	2.18	0.43
1:A:426:ILE:HG23	1:B:219:PHE:CE2	2.54	0.43
1:B:98:ARG:CB	1:B:288:ILE:HG13	2.48	0.43
2:C:85:LYS:HD3	2:C:85:LYS:HA	1.85	0.43
2:E:2:VAL:HA	2:E:26:GLY:HA3	2.01	0.43
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.18	0.43
1:A:220:ILE:HD11	1:B:434:LEU:HD11	2.00	0.43
1:B:38:MET:HA	1:B:41:VAL:HG13	2.00	0.43
2:E:123:LYS:HE2	2:E:123:LYS:HB3	1.73	0.43
1:A:337:PHE:O	1:A:341:VAL:HG23	2.19	0.43
1:A:346:LEU:O	1:A:350:SER:HB3	2.18	0.43
1:A:212:LEU:HD12	1:A:212:LEU:H	1.84	0.43
1:A:42:VAL:O	1:A:46:VAL:HG23	2.19	0.43
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.54	0.43
1:B:337:PHE:O	1:B:341:VAL:HG23	2.19	0.43
2:E:93:LEU:HD11	2:E:114:GLY:HA3	2.01	0.43
2:E:87:ARG:HH21	2:E:89:GLU:HB2	1.83	0.43
2:C:60:TYR:HE2	2:C:70:ILE:HG13	1.84	0.43
2:C:101:TYR:HB2	2:C:104:GLY:HA2	2.01	0.43
1:A:160:ARG:NE	1:A:163:LEU:HD23	2.34	0.43
1:A:98:ARG:CB	1:A:288:ILE:HG13	2.49	0.43
1:A:453:LEU:HB3	1:B:22:ILE:HG12	2.01	0.43
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.54	0.43
1:A:109:ILE:HG23	1:A:204:MET:SD	2.59	0.43
1:A:423:LEU:HD13	1:B:230:ARG:CZ	2.49	0.43
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.53	0.43
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.83	0.43
2:E:156:GLU:OE1	2:E:157:PRO:HA	2.19	0.42
1:B:235:GLU:OE1	2:C:100:TYR:HE2	2.01	0.42
1:B:330:MET:O	1:B:330:MET:HE2	2.19	0.42
1:B:147:ARG:O	1:B:151:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:O	1:B:96:LEU:HD23	2.19	0.42
1:B:46:VAL:HG22	1:B:155:GLY:HA2	2.02	0.42
1:B:360:MET:HE3	1:B:398:LEU:HD23	2.02	0.42
3:D:7:SER:HB3	3:D:8:PRO:HD3	2.00	0.42
3:D:141:LYS:HB3	3:D:172:TYR:CZ	2.55	0.42
3:D:133:CYS:HG	3:D:193:CYS:HB3	1.81	0.42
3:D:46:TRP:O	3:D:47:ILE:HG13	2.18	0.42
2:E:65:LYS:HB2	2:E:66:ASP:H	1.55	0.42
2:C:43:LYS:HB3	2:C:43:LYS:HE2	1.61	0.42
3:D:133:CYS:HB3	3:D:193:CYS:HG	1.83	0.42
3:F:6:GLN:HE21	3:F:98:GLY:C	2.23	0.42
3:D:185:TYR:CZ	3:D:210:ARG:HD2	2.55	0.42
3:D:51:SER:HB3	3:D:63:GLY:O	2.19	0.42
2:C:93:LEU:HD11	2:C:114:GLY:HA3	2.02	0.42
1:A:437:GLN:HE21	1:B:216:LYS:HZ1	1.68	0.42
1:A:75:TYR:HA	1:A:78:LEU:HD12	2.01	0.42
1:A:454:ALA:HB2	1:B:22:ILE:HG21	2.01	0.42
3:F:11:MET:HE1	3:F:19:VAL:HG13	2.02	0.42
1:A:92:PHE:O	1:A:96:LEU:HD23	2.20	0.42
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.84	0.41
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.54	0.41
1:A:434:LEU:HD23	1:B:216:LYS:HD3	2.02	0.41
1:B:160:ARG:HA	1:B:160:ARG:HD2	1.66	0.41
2:E:6:GLU:HA	2:E:22:CYS:HA	2.02	0.41
1:B:330:MET:HE2	1:B:334:VAL:HG23	2.01	0.41
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.55	0.41
3:F:115:SER:O	3:F:133:CYS:HA	2.20	0.41
1:A:227:ILE:HD11	1:B:427:ILE:HD11	2.02	0.41
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.20	0.41
1:B:171:ASP:OD2	1:B:174:ARG:NH1	2.42	0.41
3:D:95:GLN:H	3:D:95:GLN:CD	2.05	0.41
1:B:38:MET:HG3	1:B:168:LEU:HD11	2.02	0.41
1:A:171:ASP:OD2	1:A:174:ARG:NH1	2.45	0.41
2:C:194:SER:O	2:C:198:SER:OG	2.38	0.41
2:E:98:ARG:O	2:E:109:ASP:HB3	2.20	0.41
1:B:420:GLN:HG3	1:B:420:GLN:H	1.32	0.41
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.71	0.41
3:F:16:GLY:HA2	3:F:76:THR:HG23	2.01	0.41
1:A:165:ILE:HG22	1:A:166:PHE:CD2	2.56	0.41
1:A:122:VAL:HG11	1:A:160:ARG:HB2	2.02	0.41
1:A:120:ARG:NH1	1:A:452:THR:HG23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG13	1:A:244:LEU:HD21	2.03	0.41
1:B:160:ARG:HD3	1:B:160:ARG:HH11	1.76	0.41
2:E:195:SER:O	2:E:199:GLU:HB3	2.21	0.41
1:A:150:PRO:CG	1:A:354:GLY:HA2	2.51	0.41
1:B:270:ASN:HA	1:B:270:ASN:HD22	1.65	0.41
3:D:141:LYS:HB3	3:D:172:TYR:CE2	2.56	0.41
1:B:144:VAL:HG21	1:B:343:THR:OG1	2.20	0.41
3:F:8:PRO:O	3:F:101:THR:HG23	2.21	0.40
1:A:434:LEU:HA	1:A:434:LEU:HD23	1.87	0.40
1:B:346:LEU:O	1:B:350:SER:HB3	2.22	0.40
2:C:112:GLY:O	3:D:42:SER:HB3	2.21	0.40
3:D:197:HIS:CD2	3:D:198:LYS:H	2.38	0.40
2:C:30:SER:C	2:C:32:TYR:H	2.25	0.40
1:A:160:ARG:HD3	1:A:160:ARG:HH11	1.71	0.40
1:A:29:ASP:OD2	1:A:216:LYS:HE3	2.21	0.40
1:B:188:ALA:HB2	1:B:225:SER:OG	2.21	0.40
3:F:124:LEU:C	3:F:126:SER:H	2.25	0.40
3:F:29:VAL:HG11	3:F:89:GLN:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	441/446 (99%)	415 (94%)	25 (6%)	1 (0%)	52 88
1	B	439/446 (98%)	416 (95%)	22 (5%)	1 (0%)	52 88
2	C	219/222 (99%)	198 (90%)	18 (8%)	3 (1%)	14 51
2	E	219/222 (99%)	197 (90%)	19 (9%)	3 (1%)	14 51
3	D	209/211 (99%)	183 (88%)	21 (10%)	5 (2%)	7 35
3	F	209/211 (99%)	188 (90%)	20 (10%)	1 (0%)	34 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1736/1758 (99%)	1597 (92%)	125 (7%)	14 (1%)	24 66

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	B	148	ALA
2	C	140	ALA
3	D	50	THR
2	E	62	PRO
2	E	65	LYS
2	E	136	SER
3	D	76	THR
3	D	126	SER
3	F	125	THR
2	C	62	PRO
3	D	80	GLU
3	D	7	SER
2	C	157	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	333/336 (99%)	299 (90%)	34 (10%)	9 33
1	B	331/336 (98%)	301 (91%)	30 (9%)	12 41
2	C	181/182 (100%)	160 (88%)	21 (12%)	7 27
2	E	181/182 (100%)	168 (93%)	13 (7%)	18 53
3	D	185/185 (100%)	168 (91%)	17 (9%)	11 40
3	F	185/185 (100%)	168 (91%)	17 (9%)	11 40
All	All	1396/1406 (99%)	1264 (90%)	132 (10%)	11 38

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	19	ARG
1	A	65	MET
1	A	70	HIS
1	A	78	LEU
1	A	81	VAL
1	A	103	GLU
1	A	107	SER
1	A	123	ARG
1	A	136	LEU
1	A	160	ARG
1	A	180	THR
1	A	186	LEU
1	A	205	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	230	ARG
1	A	241	VAL
1	A	244	LEU
1	A	245	SER
1	A	251	THR
1	A	264	ILE
1	A	304	LEU
1	A	340	ARG
1	A	397	LEU
1	A	420	GLN
1	A	423	LEU
1	A	430	LEU
1	A	433	THR
1	A	444	LEU
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	65	MET
1	B	70	HIS
1	B	78	LEU
1	B	79	LEU
1	B	81	VAL
1	B	103	GLU
1	B	107	SER
1	B	136	LEU
1	B	160	ARG

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Mol	Chain	Res	Type
1	B	180	THR
1	B	186	LEU
1	B	205	ARG
1	B	211	THR
1	B	212	LEU
1	B	219	PHE
1	B	230	ARG
1	B	241	VAL
1	B	244	LEU
1	B	245	SER
1	B	251	THR
1	B	264	ILE
1	B	304	LEU
1	B	340	ARG
1	B	397	LEU
1	B	420	GLN
1	B	423	LEU
1	B	430	LEU
1	B	433	THR
1	B	444	LEU
1	B	453	LEU
2	C	5	LEU
2	C	7	SER
2	C	12	VAL
2	C	18	LEU
2	C	43	LYS
2	C	63	SER
2	C	66	ASP
2	C	71	SER
2	C	72	ARG
2	C	89	GLU
2	C	98	ARG
2	C	120	SER
2	C	121	SER
2	C	128	SER
2	C	142	SER
2	C	151	LYS
2	C	160	VAL
2	C	177	VAL
2	C	198	SER
2	C	204	ASN
2	C	214	VAL

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Mol	Chain	Res	Type
3	D	1	ASP
3	D	10	ILE
3	D	12	SER
3	D	51	SER
3	D	64	SER
3	D	71	SER
3	D	75	ASN
3	D	81	ASP
3	D	115	SER
3	D	120	SER
3	D	125	THR
3	D	133	CYS
3	D	135	LEU
3	D	174	MET
3	D	190	SER
3	D	192	THR
3	D	210	ARG
2	E	21	SER
2	E	30	SER
2	E	72	ARG
2	E	84	SER
2	E	87	ARG
2	E	98	ARG
2	E	115	THR
2	E	118	THR
2	E	151	LYS
2	E	186	SER
2	E	188	SER
2	E	195	SER
2	E	204	ASN
3	F	1	ASP
3	F	27	SER
3	F	39	SER
3	F	62	SER
3	F	74	ILE
3	F	77	MET
3	F	95	GLN
3	F	121	SER
3	F	125	THR
3	F	135	LEU
3	F	142	ASP
3	F	146	LYS

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Mol	Chain	Res	Type
3	F	168	LYS
3	F	170	SER
3	F	181	THR
3	F	201	THR
3	F	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	234	HIS
1	A	270	ASN
1	A	284	HIS
1	A	420	GLN
1	A	437	GLN
1	B	153	GLN
1	B	234	HIS
1	B	270	ASN
1	B	284	HIS
1	B	420	GLN
1	B	437	GLN
3	D	136	ASN
3	D	137	ASN
3	F	6	GLN
3	F	36	GLN
3	F	136	ASN
3	F	137	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	443/446 (99%)	-0.15	6 (1%)	78	51	38, 57, 83, 126	0
1	B	441/446 (98%)	-0.23	9 (2%)	68	39	37, 63, 101, 133	0
2	C	221/222 (99%)	-0.32	7 (3%)	51	23	28, 56, 91, 124	0
2	E	221/222 (99%)	-0.56	1 (0%)	91	76	34, 54, 86, 123	0
3	D	211/211 (100%)	-0.28	4 (1%)	70	41	40, 65, 89, 100	0
3	F	211/211 (100%)	-0.16	11 (5%)	31	12	31, 49, 99, 120	0
All	All	1748/1758 (99%)	-0.26	38 (2%)	65	35	28, 58, 93, 133	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	ALA	6.0
1	B	73	ASP	5.3
3	F	155	GLN	5.1
3	F	152	SER	4.0
3	F	154	ARG	3.9
3	F	149	ILE	3.9
1	A	148	ALA	3.8
1	B	74	ASN	3.8
3	F	153	GLU	3.8
2	C	29	TYR	3.5
3	F	156	ASN	3.4
1	A	459	GLU	3.4
1	A	168	LEU	3.4
1	B	71	THR	3.3
2	C	143	MET	3.3
2	C	2	VAL	3.0
2	E	222	ALA	2.9
1	B	70	HIS	2.8
3	F	151	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	2.7
3	F	127	GLY	2.7
1	A	72	ALA	2.6
3	F	150	ASP	2.5
3	D	156	ASN	2.5
3	D	68	THR	2.4
2	C	65	LYS	2.4
3	D	20	THR	2.4
2	C	141	ALA	2.3
2	C	222	ALA	2.3
1	A	440	GLY	2.3
1	B	307	PHE	2.2
3	F	147	TRP	2.2
1	B	69	VAL	2.1
1	B	75	TYR	2.1
1	B	55	LYS	2.1
3	D	159	LEU	2.1
3	F	182	LYS	2.1
2	C	64	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.