Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 10:11 AM EDT

PDB ID	:	6ELU
Title	:	Structure of Serum Resistance Associated protein from T. b. rhodesiense
Authors	:	Zoll, S.; Higgins, M.K.
Deposited on	:	2017-09-29
Resolution	:	2.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

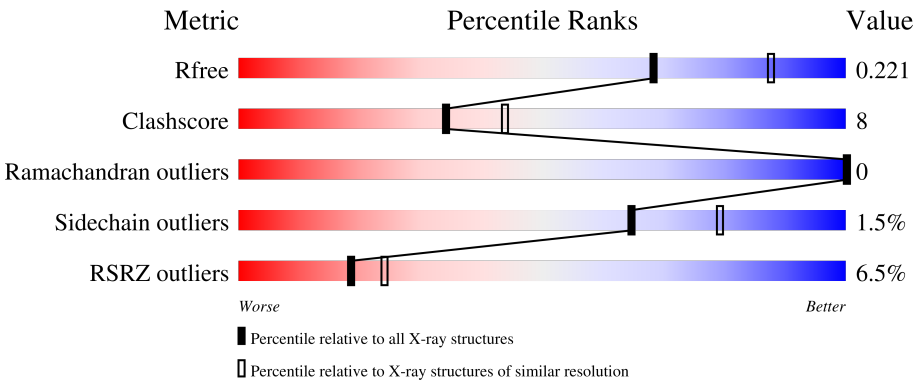
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	233	14% 60% 22% 17%
1	D	233	18% 47% 21% • 31%
1	G	233	14% 52% 19% • 28%
1	J	233	16% 52% 21% • 26%
2	B	229	% 84% 12% • •

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Mol	Chain	Length	Quality of chain
2	E	229	2% 82% 14%
2	H	229	2% 83% 14%
2	K	229	2% 82% 14%
3	C	217	90% 9%
3	F	217	91% 9%
3	I	217	89% 10%
3	L	217	92% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19153 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 Serum resistance associated; VSG protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	1413	883	247	280	3	0	0	0
1	D	161	1188	745	208	232	3	0	0	0
1	G	168	1236	775	216	242	3	0	0	0
1	J	172	1264	793	221	247	3	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q8T309
A	30	SER	-	expression tag	UNP Q8T309
A	31	HIS	-	expression tag	UNP Q8T309
A	32	MET	-	expression tag	UNP Q8T309
D	29	GLY	-	expression tag	UNP Q8T309
D	30	SER	-	expression tag	UNP Q8T309
D	31	HIS	-	expression tag	UNP Q8T309
D	32	MET	-	expression tag	UNP Q8T309
G	29	GLY	-	expression tag	UNP Q8T309
G	30	SER	-	expression tag	UNP Q8T309
G	31	HIS	-	expression tag	UNP Q8T309
G	32	MET	-	expression tag	UNP Q8T309
J	29	GLY	-	expression tag	UNP Q8T309
J	30	SER	-	expression tag	UNP Q8T309
J	31	HIS	-	expression tag	UNP Q8T309
J	32	MET	-	expression tag	UNP Q8T309

- Molecule 2 is a protein called G10_3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	222	1686	1064	280	334	8	0	0	0
2	E	222	1686	1064	280	334	8	0	0	0
2	H	222	1686	1064	280	334	8	0	0	0
2	K	222	1686	1064	280	334	8	0	0	0

- Molecule 3 is a protein called G10_3 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	217	1682	1046	282	347	7	0	0	0
3	F	217	1682	1046	282	347	7	0	0	0
3	I	217	1682	1046	282	347	7	0	0	0
3	L	217	1682	1046	282	347	7	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	1	1	0	0
4	B	49	49	49	0	0
4	C	83	83	83	0	0
4	E	50	50	50	0	0
4	F	77	77	77	0	0
4	G	4	4	4	0	0
4	H	86	86	86	0	0
4	I	91	91	91	0	0
4	J	3	3	3	0	0
4	K	74	74	74	0	0

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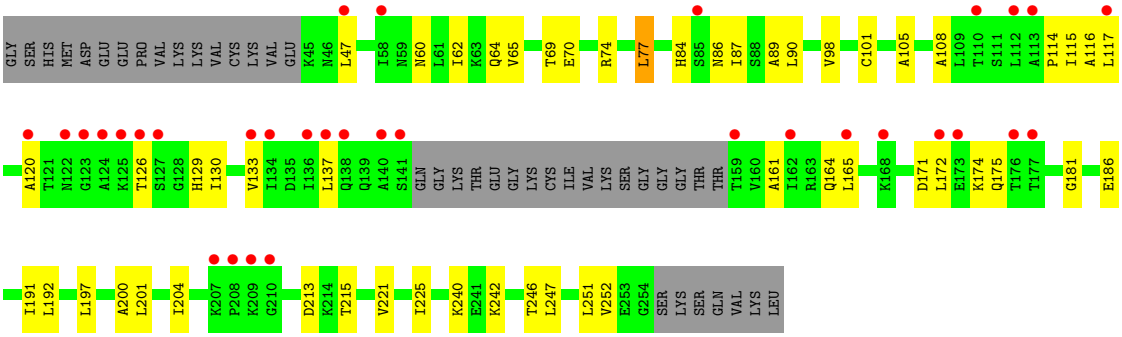
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	62	62	62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

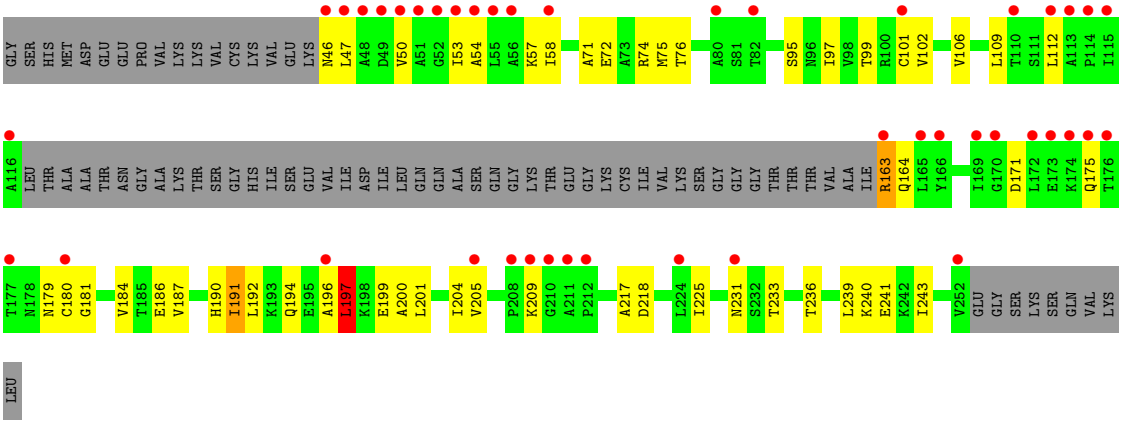
• Molecule 1: Serum resistance associated; VSG protein

Chain A:



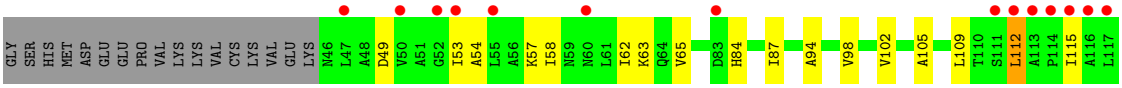
• Molecule 1: Serum resistance associated; VSG protein

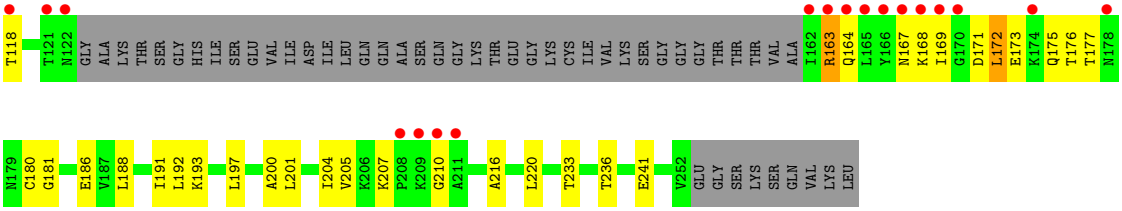
Chain D:



• Molecule 1: Serum resistance associated; VSG protein

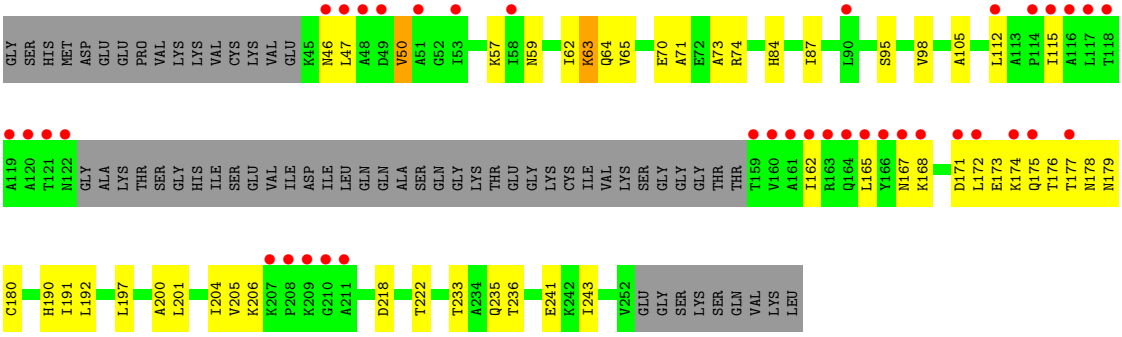
Chain G:





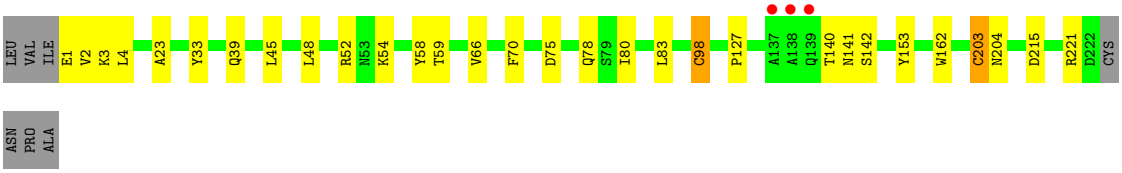
• Molecule 1: Serum resistance associated; VSG protein

Chain J:



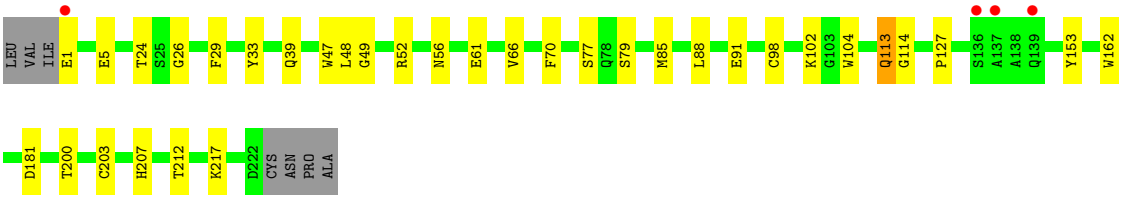
• Molecule 2: G10_3 heavy chain

Chain B:



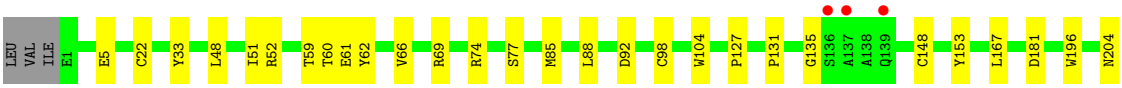
• Molecule 2: G10_3 heavy chain

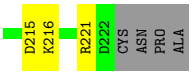
Chain E:



• Molecule 2: G10_3 heavy chain

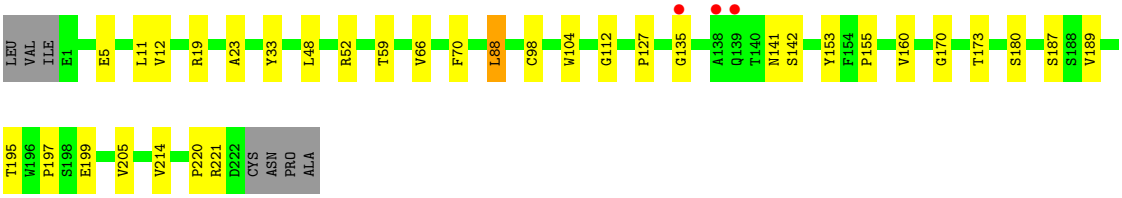
Chain H:





• Molecule 2: G10_3 heavy chain

Chain K:

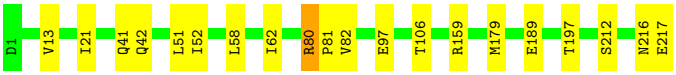


• Molecule 3: G10_3 Light chain

Chain C:

• Molecule 3: G10_3 Light chain

Chain F:



• Molecule 3: G10_3 Light chain

Chain I:

• Molecule 3: G10_3 Light chain

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.60Å 103.55Å 150.64Å 90.00° 114.58° 90.00°	Depositor
Resolution (Å)	48.43 – 2.30 48.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.43-2.30) 99.9 (48.43-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.191 , 0.220 0.191 , 0.221	Depositor DCC
R_{free} test set	7914 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19153	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.36	0/1422	0.66	2/1932 (0.1%)
1	D	0.33	0/1196	0.58	2/1625 (0.1%)
1	G	0.35	0/1244	0.64	2/1692 (0.1%)
1	J	0.41	1/1272 (0.1%)	0.64	1/1730 (0.1%)
2	B	0.40	0/1731	0.65	1/2364 (0.0%)
2	E	0.36	1/1731 (0.1%)	0.60	1/2364 (0.0%)
2	H	0.30	0/1731	0.58	0/2364
2	K	0.33	0/1731	0.61	0/2364
3	C	0.32	0/1722	0.62	2/2342 (0.1%)
3	F	0.41	2/1722 (0.1%)	0.64	4/2342 (0.2%)
3	I	0.32	0/1722	0.56	1/2342 (0.0%)
3	L	0.29	0/1722	0.53	0/2342
All	All	0.35	4/18946 (0.0%)	0.61	16/25803 (0.1%)

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
2	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	80	ARG	CG-CD	-6.22	1.36	1.51
3	F	97	GLU	CG-CD	6.13	1.61	1.51
1	J	50	VAL	CB-CG1	5.63	1.64	1.52
2	E	91	GLU	CG-CD	5.37	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	80	ARG	CG-CD-NE	-8.52	93.91	111.80
1	A	77	LEU	CB-CG-CD2	-8.48	96.58	111.00
1	D	191	ILE	CG1-CB-CG2	-8.33	93.08	111.40
1	D	197	LEU	CB-CG-CD1	-8.10	97.23	111.00
3	F	80	ARG	CA-CB-CG	-8.02	95.75	113.40
3	F	97	GLU	OE1-CD-OE2	-6.97	114.94	123.30
3	C	80	ARG	NE-CZ-NH2	-6.78	116.91	120.30
3	F	97	GLU	N-CA-CB	6.68	122.63	110.60
2	E	113	GLN	CB-CA-C	-6.66	97.08	110.40
3	F	97	GLU	CB-CA-C	-6.24	97.92	110.40
3	I	160	GLN	CA-CB-CG	-6.03	100.14	113.40
2	B	3	LYS	CG-CD-CE	-5.54	95.28	111.90
1	G	112	LEU	CB-CG-CD1	-5.50	101.66	111.00
1	J	180	CYS	CA-CB-SG	-5.14	104.75	114.00
1	A	101	CYS	CA-CB-SG	5.06	123.11	114.00
1	G	172	LEU	CB-CG-CD2	-5.05	102.42	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	140	THR	Peptide

5.2 Too-close contacts (i)

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	1413	0	1493	50	0
1	D	1188	0	1263	49	0
1	G	1236	0	1313	38	0
1	J	1264	0	1347	41	0
2	B	1686	0	1629	20	0
2	E	1686	0	1629	25	0
2	H	1686	0	1629	22	0
2	K	1686	0	1629	24	0
3	C	1682	0	1593	12	0
3	F	1682	0	1593	16	0
3	I	1682	0	1593	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1682	0	1593	9	0
4	A	1	0	0	0	0
4	B	49	0	0	0	0
4	C	83	0	0	0	0
4	E	50	0	0	1	0
4	F	77	0	0	0	0
4	G	4	0	0	1	0
4	H	86	0	0	1	0
4	I	91	0	0	1	0
4	J	3	0	0	1	0
4	K	74	0	0	2	0
4	L	62	0	0	0	0
All	All	19153	0	18304	310	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 (310) 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:161:ALA:O	1:A:164:GLN:CG	2.05	1.04
1:A:161:ALA:HA	1:A:164:GLN:HG2	1.42	1.00
3:L:193:HIS:O	3:L:215:ARG:NH2	1.94	1.00
1:A:161:ALA:O	1:A:164:GLN:HG2	1.64	0.97
1:J:192:LEU:HB3	1:J:243:ILE:HD12	1.49	0.94
1:G:57:LYS:HE2	1:G:172:LEU:HD21	1.50	0.94
1:A:161:ALA:CA	1:A:164:GLN:HG2	2.02	0.90
2:K:135:GLY:HA2	2:K:221:ARG:HD3	1.54	0.89
3:F:80:ARG:HG3	3:F:81:PRO:HA	1.55	0.85
1:A:77:LEU:O	1:A:77:LEU:HD23	1.76	0.85
1:A:161:ALA:O	1:A:164:GLN:HG3	1.73	0.85
1:J:173:GLU:HG3	1:J:174:LYS:N	1.91	0.84
1:A:161:ALA:C	1:A:164:GLN:HG2	1.98	0.83
1:A:181:GLY:HA3	1:A:186:GLU:HB3	1.60	0.83
1:G:167:ASN:O	1:G:171:ASP:N	2.11	0.82
1:D:58:ILE:HD11	1:D:112:LEU:HD11	1.62	0.81
2:K:5:GLU:OE1	2:K:23:ALA:HB3	1.81	0.80
1:A:115:ILE:O	1:A:164:GLN:NE2	2.14	0.80
1:A:164:GLN:HG3	1:A:165:LEU:N	1.99	0.78
1:D:46:ASN:HB2	1:D:163:ARG:NH2	2.00	0.77
1:A:129:HIS:O	1:A:129:HIS:ND1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:O	1:A:225:ILE:HG13	1.84	0.76
2:B:141:ASN:OD1	2:B:142:SER:N	2.19	0.76
3:I:216:ASN:O	3:I:216:ASN:ND2	2.19	0.76
1:A:98:VAL:HG23	1:A:191:ILE:HD11	1.68	0.75
1:A:171:ASP:HA	1:A:174:LYS:HD2	1.67	0.74
1:G:65:VAL:HG13	1:G:102:VAL:HG13	1.70	0.74
1:D:171:ASP:O	1:D:175:GLN:NE2	2.22	0.73
3:F:80:ARG:HG3	3:F:81:PRO:CA	2.19	0.72
1:D:233:THR:HG23	1:D:236:THR:H	1.54	0.71
1:D:46:ASN:HB2	1:D:163:ARG:HH22	1.56	0.71
1:J:167:ASN:O	1:J:171:ASP:N	2.23	0.71
1:G:57:LYS:CE	1:G:172:LEU:HD21	2.21	0.71
1:G:112:LEU:HD11	1:G:169:ILE:HG22	1.71	0.70
1:A:108:ALA:HB1	1:A:172:LEU:HD21	1.71	0.70
2:H:52:ARG:HE	2:H:59:THR:CG2	2.05	0.69
1:A:114:PRO:HB3	1:A:126:THR:HG23	1.75	0.69
2:K:195:THR:O	2:K:199:GLU:HB2	1.93	0.69
1:A:77:LEU:HD23	1:A:77:LEU:C	2.13	0.69
1:D:197:LEU:CA	1:D:199:GLU:OE2	2.40	0.68
2:B:23:ALA:HA	2:B:80:ILE:HD13	1.73	0.68
2:H:33:TYR:CE2	2:H:52:ARG:HG2	2.28	0.68
1:D:72:GLU:OE2	1:D:76:THR:HG23	1.94	0.68
2:K:141:ASN:OD1	2:K:142:SER:N	2.26	0.67
1:D:181:GLY:HA3	1:D:186:GLU:HB3	1.76	0.67
1:D:192:LEU:HA	1:D:197:LEU:HD11	1.76	0.67
2:H:52:ARG:HE	2:H:59:THR:HG23	1.58	0.67
3:F:159:ARG:NH2	3:F:189:GLU:OE2	2.21	0.67
2:E:24:THR:HG21	2:E:29:PHE:CD1	2.30	0.67
3:C:216:ASN:O	3:C:216:ASN:ND2	2.28	0.67
1:J:171:ASP:O	1:J:175:GLN:HG2	1.95	0.66
1:D:47:LEU:HD13	1:D:47:LEU:O	1.95	0.66
2:E:24:THR:HG22	2:E:79:SER:O	1.94	0.66
2:E:113:GLN:HG2	2:E:114:GLY:N	2.11	0.66
1:J:233:THR:HG23	1:J:236:THR:H	1.59	0.66
1:D:54:ALA:O	1:D:58:ILE:HD13	1.95	0.65
1:D:197:LEU:HA	1:D:199:GLU:OE2	1.97	0.65
1:J:64:GLN:NE2	4:J:301:HOH:O	2.25	0.65
3:I:40:TYR:HE1	3:I:93:GLN:HG2	1.61	0.65
2:B:4:LEU:HD23	2:B:98:CYS:SG	2.36	0.65
1:A:191:ILE:HG22	1:A:197:LEU:HD22	1.79	0.65
2:B:48:LEU:HD22	2:B:66:VAL:HG21	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:HIS:HB2	1:G:87:ILE:HG22	1.80	0.64
1:G:191:ILE:HG22	1:G:197:LEU:HD12	1.80	0.64
1:J:115:ILE:HD12	1:J:165:LEU:HA	1.79	0.63
2:H:33:TYR:CZ	2:H:52:ARG:HG2	2.33	0.62
3:L:159:ARG:NH2	3:L:189:GLU:OE1	2.33	0.61
1:A:225:ILE:HD12	1:A:240:LYS:HB2	1.83	0.61
1:J:218:ASP:O	1:J:222:THR:HG23	2.01	0.61
3:I:158:GLU:OE1	3:I:160:GLN:NE2	2.33	0.61
1:A:171:ASP:O	1:A:174:LYS:HB2	2.01	0.60
1:J:57:LYS:HE2	1:J:172:LEU:HD12	1.82	0.60
2:E:39:GLN:HE22	3:F:42:GLN:HE22	1.49	0.60
2:E:48:LEU:HD22	2:E:66:VAL:HG21	1.82	0.60
1:G:241:GLU:OE2	2:H:52:ARG:HD3	2.00	0.60
2:H:69:ARG:NH2	2:H:92:ASP:OD2	2.36	0.59
1:A:117:LEU:HD13	1:A:130:ILE:HB	1.86	0.58
2:H:85:MET:HE2	2:H:88:LEU:HD21	1.86	0.57
1:D:187:VAL:O	1:D:191:ILE:HD12	2.04	0.57
2:H:52:ARG:NH2	2:H:61:GLU:OE2	2.35	0.57
1:A:47:LEU:HG	1:A:137:LEU:HD11	1.86	0.57
3:C:41:GLN:HB2	3:C:51:LEU:HD11	1.86	0.57
3:F:41:GLN:HB2	3:F:51:LEU:HD11	1.86	0.57
1:G:175:GLN:NE2	1:G:177:THR:HG23	2.20	0.57
1:J:47:LEU:HD21	1:J:162:ILE:HD11	1.86	0.57
1:A:47:LEU:HD11	1:A:120:ALA:HA	1.88	0.56
1:A:86:ASN:N	1:A:86:ASN:OD1	2.39	0.56
2:B:54:LYS:HG3	2:B:58:TYR:CZ	2.40	0.56
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.86	0.56
2:E:33:TYR:CZ	2:E:52:ARG:HG2	2.40	0.56
1:G:163:ARG:H	1:G:163:ARG:HD3	1.69	0.56
2:K:180:SER:O	4:K:301:HOH:O	2.17	0.55
3:C:16:GLY:HA2	3:C:81:PRO:HB2	1.87	0.55
2:E:102:LYS:NZ	4:E:303:HOH:O	2.39	0.55
1:D:191:ILE:O	1:D:197:LEU:HD22	2.07	0.55
1:D:199:GLU:OE2	1:D:199:GLU:N	2.40	0.55
3:C:20:THR:HG22	3:C:78:ASN:OD1	2.06	0.54
1:A:70:GLU:O	1:A:74:ARG:HG3	2.08	0.54
1:D:241:GLU:HG2	2:E:104:TRP:HB3	1.89	0.54
1:G:207:LYS:HG3	1:G:210:GLY:H	1.72	0.54
1:A:164:GLN:HG3	1:A:165:LEU:H	1.73	0.54
3:F:52:ILE:HD13	3:F:58:LEU:HA	1.90	0.54
1:J:70:GLU:OE1	1:J:73:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:GLN:HA	1:G:167:ASN:OD1	2.08	0.54
2:K:160:VAL:HG22	2:K:205:VAL:HG22	1.90	0.53
3:F:13:VAL:HG23	3:F:82:VAL:HG21	1.90	0.53
1:D:191:ILE:HD12	1:D:191:ILE:H	1.73	0.53
2:K:12:VAL:HG11	2:K:88:LEU:HD23	1.91	0.53
2:E:52:ARG:NH2	2:E:61:GLU:OE2	2.41	0.53
1:G:115:ILE:O	1:G:118:THR:HG22	2.09	0.52
1:J:173:GLU:HG3	1:J:174:LYS:H	1.71	0.52
2:E:207:HIS:HB3	2:E:212:THR:OG1	2.08	0.52
1:G:112:LEU:HD11	1:G:169:ILE:CG2	2.39	0.52
1:G:193:LYS:O	4:G:301:HOH:O	2.19	0.52
2:H:85:MET:HB3	2:H:88:LEU:HD21	1.90	0.52
1:J:65:VAL:HG12	1:J:105:ALA:HB3	1.91	0.52
3:L:6:GLN:NE2	3:L:106:THR:HG23	2.23	0.52
3:C:112:ARG:HG3	3:C:113:ALA:O	2.10	0.52
1:A:84:HIS:HB3	1:A:86:ASN:OD1	2.10	0.51
1:D:101:CYS:CB	1:D:180:CYS:HG	2.22	0.51
1:D:71:ALA:O	1:D:75:MET:HG3	2.10	0.51
1:G:188:LEU:HA	1:G:191:ILE:HD12	1.93	0.51
2:K:48:LEU:HD22	2:K:66:VAL:HG21	1.93	0.51
2:B:1:GLU:HG3	2:B:2:VAL:N	2.25	0.51
2:E:5:GLU:HA	2:E:113:GLN:OE1	2.11	0.51
1:G:192:LEU:HA	1:G:197:LEU:HD13	1.93	0.51
1:D:191:ILE:HD12	1:D:191:ILE:N	2.26	0.51
2:E:200:THR:HG22	2:E:217:LYS:HE3	1.93	0.50
1:J:115:ILE:HD11	1:J:168:LYS:HB3	1.94	0.50
1:J:168:LYS:HA	1:J:171:ASP:HB2	1.92	0.50
3:F:13:VAL:HG21	3:F:82:VAL:HG11	1.94	0.50
1:J:233:THR:O	1:J:236:THR:HG22	2.12	0.50
1:A:192:LEU:HA	1:A:197:LEU:HD23	1.94	0.50
2:B:70:PHE:HB3	2:B:83:LEU:HD11	1.94	0.50
1:G:200:ALA:O	1:G:204:ILE:HG13	2.12	0.50
2:B:33:TYR:CZ	2:B:52:ARG:HG2	2.46	0.49
2:K:33:TYR:CE2	2:K:52:ARG:HG2	2.47	0.49
2:K:52:ARG:HD2	2:K:59:THR:OG1	2.12	0.49
3:C:112:ARG:NH1	3:C:113:ALA:O	2.45	0.49
3:I:41:GLN:HB2	3:I:51:LEU:HD11	1.94	0.49
1:A:175:GLN:OE1	1:A:175:GLN:HA	2.12	0.49
2:K:11:LEU:HB2	2:K:155:PRO:HG3	1.93	0.49
1:G:98:VAL:O	1:G:102:VAL:HG23	2.13	0.49
1:J:62:ILE:O	1:J:65:VAL:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:ALA:O	1:J:204:ILE:HG13	2.13	0.49
2:E:85:MET:HB3	2:E:88:LEU:HD21	1.94	0.49
2:K:173:THR:HG22	2:K:187:SER:OG	2.13	0.49
1:A:84:HIS:HB2	1:A:87:ILE:HG22	1.93	0.48
2:B:66:VAL:HG13	2:B:70:PHE:HB2	1.94	0.48
1:G:191:ILE:HG22	1:G:197:LEU:CD1	2.43	0.48
1:G:241:GLU:HG2	2:H:104:TRP:HB3	1.95	0.48
3:C:165:ASN:HB3	3:C:179:MET:HE1	1.94	0.48
1:G:49:ASP:O	1:G:53:ILE:HD13	2.14	0.48
1:A:137:LEU:HD13	1:A:137:LEU:O	2.13	0.48
1:A:213:ASP:OD1	1:A:215:THR:HG22	2.13	0.48
1:J:50:VAL:CG1	1:J:165:LEU:HD22	2.43	0.48
1:J:192:LEU:HA	1:J:197:LEU:HD23	1.94	0.48
1:G:181:GLY:HA3	1:G:186:GLU:HB3	1.95	0.48
2:H:48:LEU:HD22	2:H:66:VAL:HG11	1.96	0.48
1:D:200:ALA:O	1:D:204:ILE:HG13	2.14	0.48
1:J:59:ASN:HB3	1:J:63:LYS:NZ	2.28	0.48
2:K:127:PRO:HB3	2:K:153:TYR:HB3	1.95	0.48
1:D:101:CYS:CB	1:D:180:CYS:SG	3.02	0.48
1:D:194:GLN:O	1:D:197:LEU:HD23	2.14	0.48
1:D:233:THR:HG23	1:D:236:THR:N	2.27	0.48
1:J:191:ILE:HG22	1:J:197:LEU:HD22	1.96	0.48
1:J:178:ASN:O	1:J:190:HIS:NE2	2.46	0.47
2:K:33:TYR:CZ	2:K:52:ARG:HG2	2.49	0.47
2:K:112:GLY:O	3:L:47:PRO:HB3	2.14	0.47
2:B:75:ASP:CG	2:B:78:GLN:HG3	2.35	0.47
3:I:18:ARG:NH2	3:I:80:ARG:HD3	2.28	0.47
1:G:65:VAL:HG22	1:G:105:ALA:HB3	1.97	0.47
1:J:46:ASN:O	1:J:50:VAL:HG23	2.15	0.47
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.95	0.47
1:A:130:ILE:O	1:A:133:VAL:HG12	2.14	0.47
1:D:197:LEU:N	1:D:199:GLU:OE2	2.49	0.46
2:H:135:GLY:HA2	2:H:221:ARG:HD3	1.96	0.46
2:K:205:VAL:HB	2:K:214:VAL:HG13	1.97	0.46
1:J:50:VAL:HG11	1:J:165:LEU:HD22	1.97	0.46
3:F:197:THR:HG22	3:F:212:SER:CB	2.46	0.46
3:F:197:THR:HG22	3:F:212:SER:HB3	1.96	0.46
1:A:161:ALA:HA	1:A:164:GLN:CG	2.29	0.46
1:D:192:LEU:C	1:D:197:LEU:HD21	2.35	0.46
1:D:180:CYS:HB3	1:D:190:HIS:CG	2.51	0.46
1:D:201:LEU:O	1:D:205:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:203:LYS:NZ	4:I:307:HOH:O	2.47	0.46
2:K:66:VAL:HG13	2:K:70:PHE:HB2	1.97	0.46
2:B:54:LYS:HG3	2:B:58:TYR:OH	2.16	0.46
1:D:102:VAL:O	1:D:106:VAL:HG12	2.16	0.46
3:I:217:GLU:N	3:I:217:GLU:OE1	2.49	0.46
2:K:19:ARG:NH1	4:K:309:HOH:O	2.39	0.46
1:D:225:ILE:HG21	1:D:236:THR:HG23	1.98	0.45
3:C:199:GLU:HG2	3:C:210:VAL:HG22	1.97	0.45
1:D:95:SER:O	1:D:99:THR:HG23	2.16	0.45
1:G:201:LEU:O	1:G:205:VAL:HG22	2.16	0.45
1:J:233:THR:CG2	1:J:236:THR:H	2.29	0.45
2:E:39:GLN:HE22	3:F:42:GLN:NE2	2.13	0.45
3:I:159:ARG:NH2	3:I:189:GLU:OE2	2.46	0.45
3:C:197:THR:HG22	3:C:212:SER:HB3	1.99	0.45
1:A:65:VAL:O	1:A:69:THR:HG23	2.17	0.45
2:E:33:TYR:CE2	2:E:52:ARG:HG2	2.51	0.45
2:K:197:PRO:HB3	2:K:220:PRO:HG3	1.99	0.45
1:A:89:ALA:HB3	1:A:204:ILE:HD11	1.99	0.44
1:G:57:LYS:HD2	1:G:57:LYS:HA	1.55	0.44
1:J:95:SER:HA	1:J:98:VAL:HG12	1.99	0.44
1:A:108:ALA:HB1	1:A:172:LEU:CD2	2.43	0.44
1:A:116:ALA:HB3	1:A:130:ILE:HD11	1.99	0.44
1:D:97:ILE:HD11	1:D:196:ALA:HB3	1.99	0.44
2:B:23:ALA:CA	2:B:80:ILE:HD13	2.46	0.44
1:A:77:LEU:C	1:A:77:LEU:CD2	2.86	0.44
1:D:192:LEU:O	1:D:197:LEU:HD21	2.17	0.44
3:F:21:ILE:HG12	3:F:106:THR:HG21	1.98	0.44
2:B:33:TYR:CE2	2:B:52:ARG:HG2	2.53	0.43
1:G:94:ALA:O	1:G:98:VAL:HG13	2.18	0.43
1:J:233:THR:H	1:J:236:THR:HG22	1.82	0.43
2:E:66:VAL:HG13	2:E:70:PHE:CG	2.53	0.43
1:G:58:ILE:O	1:G:62:ILE:HD13	2.18	0.43
1:J:71:ALA:HB3	1:J:98:VAL:HG21	2.00	0.43
1:A:116:ALA:HA	1:A:165:LEU:HD22	2.00	0.43
1:G:57:LYS:HE2	1:G:172:LEU:CD2	2.35	0.43
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.54	0.43
1:G:216:ALA:O	1:G:220:LEU:HG	2.18	0.43
3:I:144:TYR:CG	3:I:145:PRO:HA	2.53	0.43
1:A:62:ILE:O	1:A:65:VAL:HG22	2.18	0.43
3:F:58:LEU:HD21	3:F:62:ILE:O	2.18	0.43
2:H:51:ILE:HD13	2:H:74:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:ASN:OD1	1:J:46:ASN:N	2.50	0.43
2:B:52:ARG:NH1	2:B:59:THR:OG1	2.49	0.43
1:D:205:VAL:HG11	1:D:217:ALA:HB2	2.00	0.43
1:D:239:LEU:O	1:D:243:ILE:HD12	2.19	0.43
2:H:127:PRO:HB3	2:H:153:TYR:HB3	2.01	0.43
3:I:13:VAL:HG12	3:I:108:LEU:HD11	1.99	0.43
1:A:242:LYS:O	1:A:246:THR:HG23	2.18	0.43
2:H:167:LEU:HD23	2:H:167:LEU:HA	1.90	0.43
1:J:84:HIS:HB2	1:J:87:ILE:HG22	2.00	0.43
3:L:95:SER:HA	3:L:100:TRP:CE3	2.53	0.43
1:D:192:LEU:HD23	1:D:197:LEU:HD11	2.01	0.43
2:H:60:THR:HG1	2:H:62:TYR:HE2	1.65	0.43
2:B:204:ASN:ND2	2:B:215:ASP:OD1	2.45	0.43
1:A:225:ILE:CD1	1:A:240:LYS:HB2	2.47	0.42
1:D:240:LYS:HE3	2:E:56:ASN:OD1	2.19	0.42
2:H:196:TRP:O	4:H:301:HOH:O	2.21	0.42
1:D:187:VAL:O	1:D:191:ILE:CD1	2.66	0.42
1:A:47:LEU:HG	1:A:137:LEU:CD1	2.48	0.42
1:D:191:ILE:HG22	1:D:197:LEU:HD13	2.01	0.42
3:C:126:SER:O	3:C:130:THR:HG23	2.19	0.42
3:C:201:THR:HG22	3:C:208:PRO:HB3	2.01	0.42
2:K:66:VAL:HG13	2:K:70:PHE:CG	2.54	0.42
1:A:200:ALA:O	1:A:204:ILE:HG13	2.19	0.42
1:A:247:LEU:O	1:A:251:LEU:HD12	2.19	0.42
1:D:50:VAL:HG13	1:D:163:ARG:NH1	2.34	0.42
1:G:164:GLN:O	1:G:168:LYS:N	2.51	0.42
1:J:70:GLU:OE1	1:J:74:ARG:HG2	2.20	0.42
1:D:101:CYS:HB3	1:D:180:CYS:SG	2.60	0.42
1:D:225:ILE:HD13	1:D:240:LYS:HB2	2.01	0.42
2:E:1:GLU:O	2:E:26:GLY:HA3	2.19	0.42
2:H:131:PRO:HD3	2:H:216:LYS:HG2	2.02	0.42
3:I:122:PHE:HA	3:I:123:PRO:HD3	1.94	0.42
3:C:112:ARG:HG3	3:C:112:ARG:HH11	1.84	0.42
3:F:80:ARG:CG	3:F:81:PRO:N	2.81	0.42
1:G:233:THR:H	1:G:236:THR:HB	1.85	0.42
2:B:39:GLN:HB2	2:B:45:LEU:HD23	2.02	0.42
1:G:62:ILE:HD12	1:G:109:LEU:HD11	2.02	0.42
1:J:173:GLU:O	1:J:177:THR:HG23	2.20	0.42
1:J:235:GLN:OE1	1:J:235:GLN:N	2.47	0.42
1:A:65:VAL:HG12	1:A:105:ALA:HB3	2.01	0.41
1:D:109:LEU:HD23	1:D:109:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:39:GLN:NE2	3:F:42:GLN:HE22	2.16	0.41
3:F:216:ASN:O	3:F:217:GLU:HG3	2.20	0.41
2:K:170:GLY:O	2:K:189:VAL:HA	2.20	0.41
3:L:179:MET:HG2	3:L:180:SER:N	2.34	0.41
1:D:218:ASP:CG	1:D:240:LYS:HZ1	2.23	0.41
2:H:216:LYS:HE2	3:I:127:GLU:OE1	2.19	0.41
1:A:252:VAL:HG12	1:A:252:VAL:O	2.19	0.41
1:D:187:VAL:CG1	1:D:191:ILE:HD11	2.51	0.41
1:G:63:LYS:HD3	1:G:63:LYS:HA	1.78	0.41
3:L:199:GLU:HG2	3:L:210:VAL:HG22	2.01	0.41
2:B:162:TRP:CZ3	2:B:203:CYS:HB3	2.55	0.41
1:D:74:ARG:HH21	1:D:184:VAL:HG21	1.85	0.41
3:I:199:GLU:HG2	3:I:210:VAL:HG12	2.02	0.41
1:J:59:ASN:HB3	1:J:63:LYS:HZ2	1.85	0.41
3:L:191:GLU:C	3:L:215:ARG:NH2	2.74	0.41
1:D:50:VAL:HG13	1:D:163:ARG:HH12	1.86	0.41
1:D:187:VAL:HG12	1:D:191:ILE:CD1	2.51	0.41
2:H:85:MET:HE2	2:H:88:LEU:CD2	2.50	0.41
1:G:115:ILE:HA	1:G:118:THR:HG22	2.03	0.41
1:G:168:LYS:HA	1:G:171:ASP:HB2	2.03	0.41
1:A:90:LEU:HD21	1:A:201:LEU:HB2	2.03	0.41
2:E:24:THR:CG2	2:E:79:SER:HB3	2.49	0.41
1:J:70:GLU:OE1	1:J:70:GLU:O	2.39	0.41
1:A:60:ASN:O	1:A:64:GLN:HG3	2.21	0.41
3:I:18:ARG:NH2	3:I:80:ARG:HH11	2.19	0.41
2:K:5:GLU:O	2:K:5:GLU:HG2	2.19	0.41
2:B:66:VAL:HG13	2:B:70:PHE:CG	2.56	0.41
2:E:113:GLN:HG2	2:E:114:GLY:H	1.86	0.41
2:E:127:PRO:HB3	2:E:153:TYR:HB3	2.03	0.41
1:J:241:GLU:HG2	2:K:104:TRP:HB3	2.03	0.41
2:B:66:VAL:CG1	2:B:70:PHE:HB2	2.52	0.40
1:J:176:THR:O	1:J:179:ASN:HB3	2.21	0.40
2:K:141:ASN:CG	2:K:142:SER:N	2.75	0.40
1:D:53:ILE:HD12	1:D:54:ALA:N	2.35	0.40
2:H:5:GLU:O	2:H:22:CYS:HA	2.21	0.40
1:J:178:ASN:OD1	1:J:178:ASN:N	2.54	0.40
1:G:176:THR:O	1:G:176:THR:HG22	2.20	0.40
1:J:233:THR:H	1:J:236:THR:CG2	2.33	0.40
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.57	0.40
2:E:66:VAL:HG13	2:E:70:PHE:HB2	2.03	0.40
2:H:204:ASN:ND2	2:H:215:ASP:OD1	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:ALA:O	1:G:57:LYS:HB3	2.22	0.40
1:J:201:LEU:O	1:J:205:VAL:HG22	2.21	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	189/233 (81%)	185 (98%)	4 (2%)	0	100	100
1	D	157/233 (67%)	153 (98%)	4 (2%)	0	100	100
1	G	164/233 (70%)	160 (98%)	4 (2%)	0	100	100
1	J	168/233 (72%)	163 (97%)	5 (3%)	0	100	100
2	B	220/229 (96%)	215 (98%)	5 (2%)	0	100	100
2	E	220/229 (96%)	215 (98%)	5 (2%)	0	100	100
2	H	220/229 (96%)	216 (98%)	4 (2%)	0	100	100
2	K	220/229 (96%)	215 (98%)	5 (2%)	0	100	100
3	C	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
3	F	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
3	I	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
3	L	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
All	All	2418/2716 (89%)	2357 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/188 (82%)	154 (100%)	0	100	100
1	D	130/188 (69%)	123 (95%)	7 (5%)	22	30
1	G	135/188 (72%)	132 (98%)	3 (2%)	52	69
1	J	138/188 (73%)	135 (98%)	3 (2%)	52	69
2	B	188/194 (97%)	185 (98%)	3 (2%)	62	78
2	E	188/194 (97%)	185 (98%)	3 (2%)	62	78
2	H	188/194 (97%)	184 (98%)	4 (2%)	53	70
2	K	188/194 (97%)	186 (99%)	2 (1%)	73	86
3	C	190/190 (100%)	187 (98%)	3 (2%)	62	78
3	F	190/190 (100%)	189 (100%)	1 (0%)	88	95
3	I	190/190 (100%)	188 (99%)	2 (1%)	73	86
3	L	190/190 (100%)	189 (100%)	1 (0%)	88	95
All	All	2069/2288 (90%)	2037 (98%)	32 (2%)	65	79

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	98	CYS
2	B	203	CYS
2	B	221	ARG
3	C	80	ARG
3	C	159	ARG
3	C	179	MET
1	D	57	LYS
1	D	163	ARG
1	D	164	GLN
1	D	179	ASN
1	D	197	LEU
1	D	209	LYS
1	D	231	ASN
2	E	77	SER

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Mol	Chain	Res	Type
2	E	98	CYS
2	E	181	ASP
3	F	179	MET
1	G	163	ARG
1	G	173	GLU
1	G	180	CYS
2	H	77	SER
2	H	98	CYS
2	H	148	CYS
2	H	181	ASP
3	I	73	THR
3	I	93	GLN
1	J	63	LYS
1	J	112	LEU
1	J	206	LYS
2	K	88	LEU
2	K	98	CYS
3	L	94	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	175	GLN
2	E	13	GLN
2	E	39	GLN
2	E	139	GLN
3	F	149	ASN
3	L	216	ASN

5.3.3 RNA (i)

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	193/233 (82%)	0.83	33 (17%)	1	2	65, 98, 165, 185	0
1	D	161/233 (69%)	1.19	43 (26%)	0	0	74, 113, 188, 213	0
1	G	168/233 (72%)	0.76	32 (19%)	1	1	53, 97, 177, 196	0
1	J	172/233 (73%)	0.95	38 (22%)	0	1	49, 94, 183, 210	0
2	B	222/229 (96%)	-0.11	3 (1%)	75	80	32, 58, 101, 148	0
2	E	222/229 (96%)	-0.11	4 (1%)	68	74	30, 54, 88, 141	1 (0%)
2	H	222/229 (96%)	-0.23	3 (1%)	75	80	32, 51, 90, 170	1 (0%)
2	K	222/229 (96%)	-0.23	3 (1%)	75	80	35, 52, 88, 165	0
3	C	217/217 (100%)	-0.26	0	100	100	32, 52, 84, 122	0
3	F	217/217 (100%)	-0.28	0	100	100	31, 51, 86, 114	0
3	I	217/217 (100%)	-0.30	0	100	100	30, 47, 79, 145	0
3	L	217/217 (100%)	-0.19	0	100	100	36, 56, 103, 152	0
All	All	2450/2716 (90%)	0.11	159 (6%)	18	24	30, 60, 156, 213	2 (0%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	PRO	10.9
1	D	48	ALA	9.1
1	J	209	LYS	8.0
1	G	166	TYR	7.6
1	D	210	GLY	7.1
1	A	209	LYS	7.0
1	A	210	GLY	7.0
1	J	112	LEU	6.9
1	J	208	PRO	6.8
1	D	112	LEU	6.7
1	D	173	GLU	6.4

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Mol	Chain	Res	Type	RSRZ
1	J	117	LEU	6.4
1	G	50	VAL	6.4
2	H	137	ALA	6.2
2	B	137	ALA	6.1
1	D	50	VAL	6.0
1	J	211	ALA	5.8
1	G	116	ALA	5.8
1	J	47	LEU	5.7
1	D	54	ALA	5.7
1	G	47	LEU	5.7
1	G	121	THR	5.7
1	D	56	ALA	5.6
1	G	164	GLN	5.4
1	J	166	TYR	5.3
1	D	166	TYR	5.1
1	J	163	ARG	5.1
1	G	112	LEU	5.1
1	D	175	GLN	5.1
1	A	162	ILE	5.0
1	G	122	ASN	5.0
1	J	118	THR	4.9
1	D	49	ASP	4.9
1	D	163	ARG	4.8
1	J	175	GLN	4.8
1	A	172	LEU	4.8
1	D	205	VAL	4.7
1	D	196	ALA	4.6
1	D	53	ILE	4.5
1	J	120	ALA	4.5
1	A	208	PRO	4.5
1	J	161	ALA	4.5
1	J	174	LYS	4.4
1	G	163	ARG	4.3
1	J	121	THR	4.3
1	J	162	ILE	4.3
1	A	124	ALA	4.3
1	A	125	LYS	4.2
1	A	177	THR	4.1
1	A	140	ALA	4.1
1	D	58	ILE	4.0
2	E	137	ALA	4.0
1	G	53	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	139	GLN	4.0
1	D	211	ALA	4.0
1	D	113	ALA	3.9
1	A	133	VAL	3.9
1	J	116	ALA	3.9
1	D	110	THR	3.9
1	J	160	VAL	3.9
1	J	51	ALA	3.9
1	J	53	ILE	3.8
1	D	52	GLY	3.8
1	G	174	LYS	3.7
1	D	55	LEU	3.7
1	A	117	LEU	3.6
1	D	208	PRO	3.6
1	G	165	LEU	3.6
1	G	162	ILE	3.6
1	A	176	THR	3.6
1	G	117	LEU	3.6
1	D	177	THR	3.5
1	A	58	ILE	3.5
1	D	209	LYS	3.4
1	G	178	ASN	3.4
1	A	113	ALA	3.3
1	J	168	LYS	3.3
1	A	137	LEU	3.3
1	D	174	LYS	3.3
1	G	118	THR	3.2
1	J	119	ALA	3.2
1	J	164	GLN	3.2
1	G	168	LYS	3.1
1	A	112	LEU	3.1
1	J	115	ILE	3.1
2	E	139	GLN	3.1
1	G	170	GLY	3.1
2	B	138	ALA	3.1
1	J	165	LEU	3.0
1	A	141	SER	3.0
1	D	80	ALA	2.9
1	J	167	ASN	2.9
1	G	211	ALA	2.9
1	D	47	LEU	2.9
1	J	159	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	49	ASP	2.8
1	D	82	THR	2.8
1	J	48	ALA	2.8
1	G	114	PRO	2.8
1	G	209	LYS	2.8
1	J	172	LEU	2.7
1	A	126	THR	2.7
1	D	176	THR	2.7
1	A	165	LEU	2.7
1	G	169	ILE	2.7
1	A	138	GLN	2.7
1	J	46	ASN	2.7
1	J	207	LYS	2.7
1	A	47	LEU	2.7
2	H	136	SER	2.6
1	G	115	ILE	2.6
1	G	60	ASN	2.6
2	K	139	GLN	2.6
1	A	123	GLY	2.5
1	J	90	LEU	2.5
1	G	55	LEU	2.5
1	D	172	LEU	2.4
1	A	159	THR	2.4
2	E	136	SER	2.4
1	A	122	ASN	2.4
1	J	114	PRO	2.4
1	D	231	ASN	2.4
1	G	52	GLY	2.3
1	A	134	ILE	2.3
2	E	1	GLU	2.3
1	G	208	PRO	2.3
1	J	122	ASN	2.3
2	K	138	ALA	2.3
1	J	171	ASP	2.3
1	D	170	GLY	2.3
1	G	167	ASN	2.3
1	D	101	CYS	2.3
1	A	85	SER	2.3
1	D	169	ILE	2.3
1	G	83	ASP	2.2
1	G	113	ALA	2.2
1	D	46	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	139	GLN	2.2
1	D	212	PRO	2.2
1	G	210	GLY	2.2
1	A	136	ILE	2.1
1	D	180	CYS	2.1
1	A	127	SER	2.1
1	D	116	ALA	2.1
1	D	115	ILE	2.1
1	A	168	LYS	2.1
1	D	252	VAL	2.1
1	A	173	GLU	2.1
1	J	58	ILE	2.1
1	J	210	GLY	2.1
1	A	120	ALA	2.1
1	D	51	ALA	2.1
1	G	111	SER	2.1
2	K	135	GLY	2.1
1	D	224	LEU	2.1
1	A	207	LYS	2.1
1	D	165	LEU	2.0
1	A	110	THR	2.0
1	J	177	THR	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 monosaccharides 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.