Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 09:50 pm GMT

PDB ID	:	2J1K
Title	:	CAV-2 fibre head in complex with CAR D1
Authors	:	Seiradake, E.; Lortat-Jacob, H.; Billet, O.; Kremer, E.J.; Cusack, S.
Deposited on	:	2006-08-14
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:

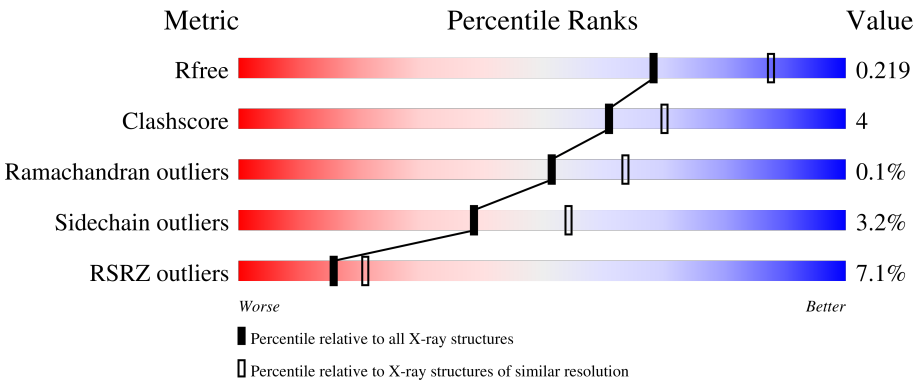
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	128	28% 75% 14% • 9%
1	B	128	37% 63% 23% • 12%
1	G	128	5% 80% 14% • •
1	J	128	5% 82% 13% • •
1	K	128	4% 82% 13% • •

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Mol	Chain	Length	Quality of chain
1	O	128	3% 73% 18% 8%
1	P	128	9% 84% 10%
1	T	128	9% 76% 14% 7%
1	V	128	23% 78% 16% 5%
1	X	128	7% 80% 16%
1	Y	128	19% 75% 16% 7%
1	Z	128	34% 73% 16% 9%
2	C	197	86% 6% 8%
2	D	197	3% 85% 7% 8%
2	E	197	% 86% 7% 8%
2	F	197	86% 6% 8%
2	H	197	85% 7% 8%
2	I	197	87% 6% 8%
2	L	197	2% 84% 8% 8%
2	M	197	2% 85% 7% 8%
2	N	197	84% 8% 8%
2	Q	197	6% 84% 8% 8%
2	R	197	88% 5% 8%
2	S	197	85% 7% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29978 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 COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	117	914	581	147	183	3	0	0	0
1	B	113	881	565	142	171	3	0	0	0
1	G	123	959	611	156	189	3	0	0	0
1	J	123	959	611	156	189	3	0	0	0
1	K	123	963	615	156	189	3	0	0	0
1	O	118	917	587	145	182	3	0	0	0
1	P	123	959	611	156	189	3	0	0	0
1	T	119	928	591	149	185	3	0	0	0
1	V	121	944	600	154	187	3	0	0	0
1	X	123	959	611	156	189	3	0	0	0
1	Y	119	928	591	149	185	3	0	0	0
1	Z	117	914	581	147	183	3	0	0	0

- Molecule 2 is a protein called FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	182	1406	892	239	266	9	0	0	0
2	D	182	1406	892	239	266	9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	182	1406	892	239	266	9	0	0	0
2	F	182	1406	892	239	266	9	0	0	0
2	H	182	1406	892	239	266	9	0	0	0
2	I	182	1406	892	239	266	9	0	0	0
2	L	182	1406	892	239	266	9	0	0	0
2	M	182	1406	892	239	266	9	0	0	0
2	N	182	1406	892	239	266	9	0	0	0
2	Q	182	1406	892	239	266	9	0	0	0
2	R	182	1406	892	239	266	9	0	0	0
2	S	182	1406	892	239	266	9	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	24	24	24	0	0
3	B	15	15	15	0	0
3	C	140	140	140	0	0
3	D	127	127	127	0	0
3	E	121	121	121	0	0
3	F	129	129	129	0	0
3	G	53	53	53	0	0
3	H	135	135	135	0	0
3	I	148	148	148	0	0

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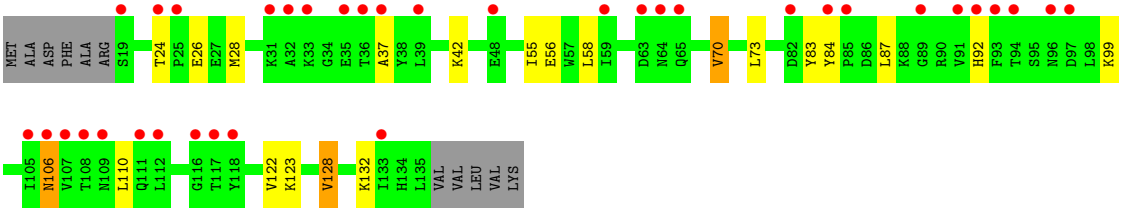
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	45	Total O 45 45	0	0
3	K	45	Total O 45 45	0	0
3	L	116	Total O 116 116	0	0
3	M	134	Total O 134 134	0	0
3	N	118	Total O 118 118	0	0
3	O	31	Total O 31 31	0	0
3	P	54	Total O 54 54	0	0
3	Q	101	Total O 101 101	0	0
3	R	111	Total O 111 111	0	0
3	S	93	Total O 93 93	0	0
3	T	32	Total O 32 32	0	0
3	V	23	Total O 23 23	0	0
3	X	50	Total O 50 50	0	0
3	Y	23	Total O 23 23	0	0
3	Z	13	Total O 13 13	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.

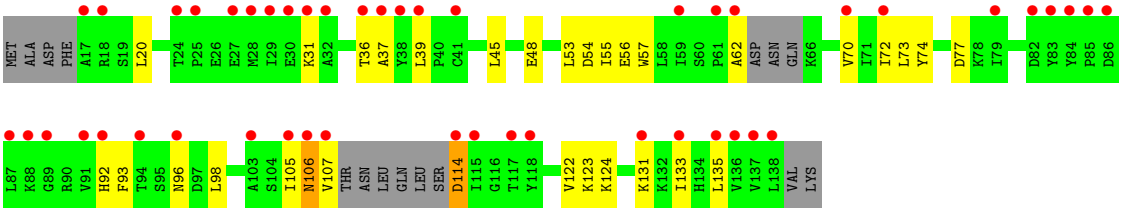
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain A:



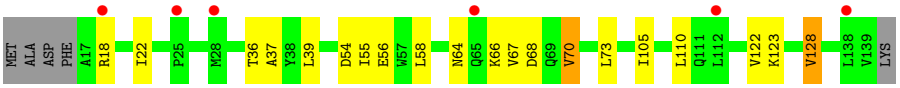
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain B:



• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain G:

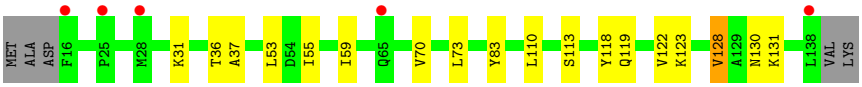


• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain J:

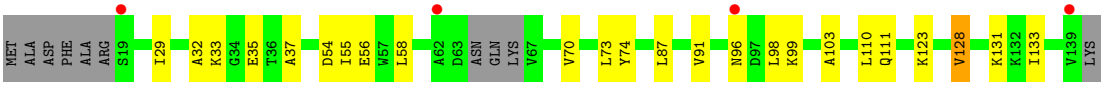
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain K:



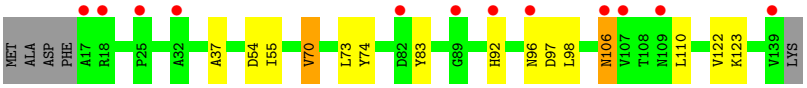
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain O:



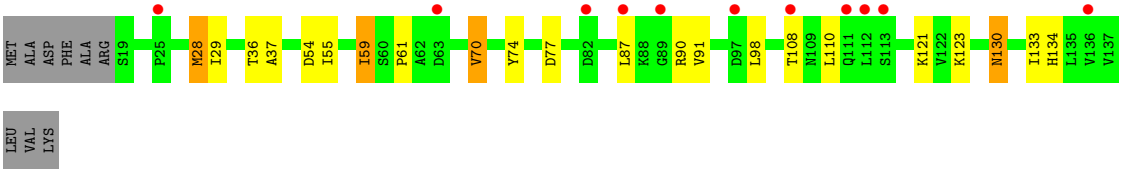
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain P:



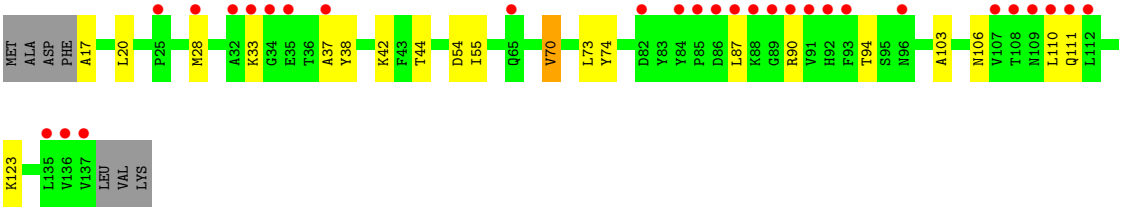
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain T:



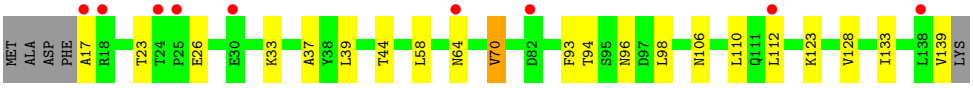
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain V:



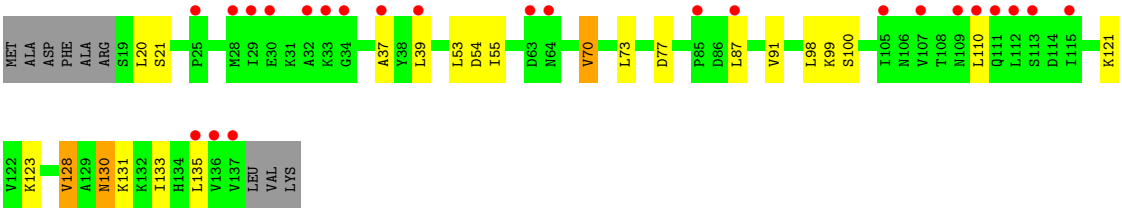
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain X:



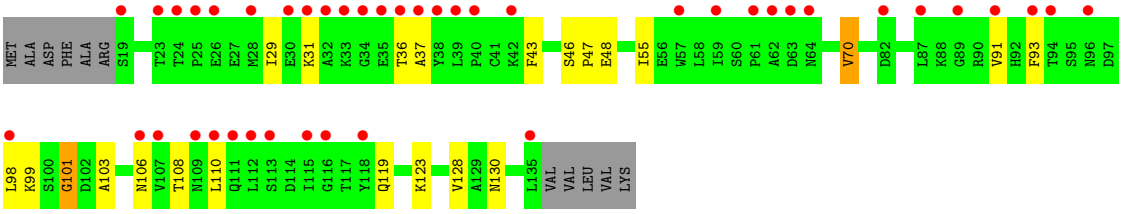
• Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain Y:



- Molecule 1: COXSACKIEVIRUS AND ADENOVIRUS RECEPTOR

Chain Z:

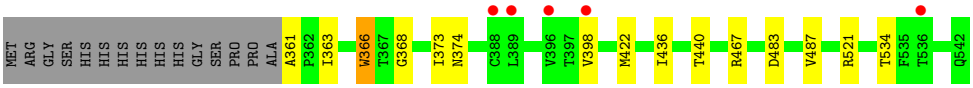


- Molecule 2: FIBER PROTEIN

Chain C:

- Molecule 2: FIBER PROTEIN

Chain D:



- Molecule 2: FIBER PROTEIN

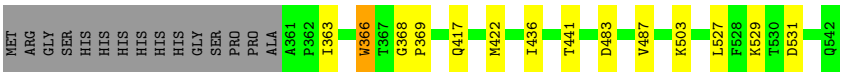
Chain E:

- Molecule 2: FIBER PROTEIN

Chain F:

- Molecule 2: FIBER PROTEIN

Chain H:

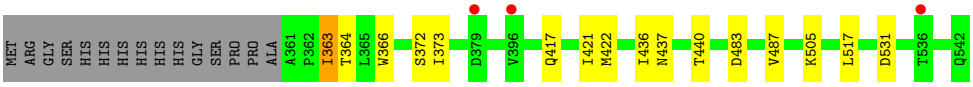


• Molecule 2: FIBER PROTEIN

Chain I:

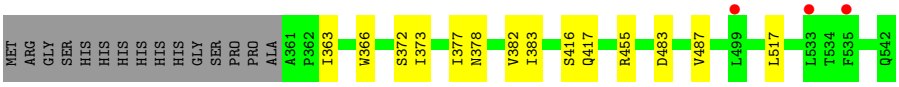
• Molecule 2: FIBER PROTEIN

Chain L:



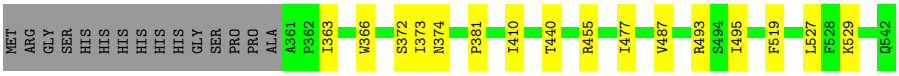
• Molecule 2: FIBER PROTEIN

Chain M:



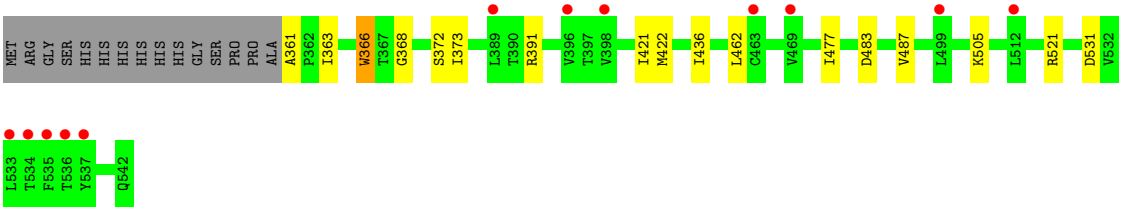
• Molecule 2: FIBER PROTEIN

Chain N:



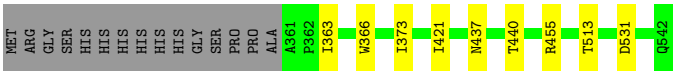
• Molecule 2: FIBER PROTEIN

Chain Q:



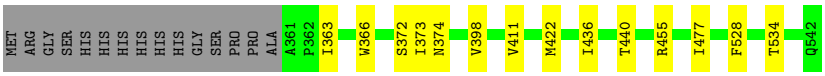
• Molecule 2: FIBER PROTEIN

Chain R:



• Molecule 2: FIBER PROTEIN

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	219.94Å 219.94Å 387.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	192.45 – 2.30 47.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (192.45-2.30) 92.0 (47.67-2.30)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.220 0.172 , 0.219	Depositor DCC
R_{free} test set	1890 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29978	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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	0.37	0/932	0.57	0/1264
1	B	0.78	3/897 (0.3%)	0.63	1/1213 (0.1%)
1	G	0.43	0/977	0.64	0/1326
1	J	0.44	0/977	0.61	0/1326
1	K	0.43	0/982	0.61	0/1332
1	O	0.44	0/934	0.60	0/1268
1	P	0.40	0/977	0.61	0/1326
1	T	0.41	0/946	0.60	0/1284
1	V	0.38	0/962	0.55	0/1305
1	X	0.42	0/977	0.59	0/1326
1	Y	0.38	0/946	0.56	0/1284
1	Z	0.36	0/932	0.52	0/1264
2	C	0.50	0/1441	0.68	0/1964
2	D	0.51	0/1441	0.68	0/1964
2	E	0.51	0/1441	0.66	0/1964
2	F	0.52	0/1441	0.67	0/1964
2	H	0.53	0/1441	0.65	0/1964
2	I	0.50	0/1441	0.65	0/1964
2	L	0.48	0/1441	0.64	0/1964
2	M	0.51	0/1441	0.63	0/1964
2	N	0.47	0/1441	0.63	0/1964
2	Q	0.46	0/1441	0.63	0/1964
2	R	0.45	0/1441	0.65	0/1964
2	S	0.46	0/1441	0.62	0/1964
All	All	0.48	3/28731 (0.0%)	0.63	1/39086 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	ALA	C-O	16.91	1.55	1.23
1	B	114	ASP	CG-OD1	7.06	1.41	1.25
1	B	114	ASP	CG-OD2	6.25	1.39	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	114	ASP	CB-CG-OD2	-6.11	112.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	914	0	910	13	0
1	B	881	0	889	22	0
1	G	959	0	966	15	0
1	J	959	0	966	10	0
1	K	963	0	966	13	0
1	O	917	0	920	21	0
1	P	959	0	966	14	0
1	T	928	0	928	16	0
1	V	944	0	946	14	0
1	X	959	0	966	13	0
1	Y	928	0	928	17	0
1	Z	914	0	910	13	0
2	C	1406	0	1382	9	0
2	D	1406	0	1382	10	0
2	E	1406	0	1382	9	0
2	F	1406	0	1382	8	0
2	H	1406	0	1382	8	0
2	I	1406	0	1382	6	0
2	L	1406	0	1382	10	0
2	M	1406	0	1382	6	0
2	N	1406	0	1382	10	0
2	Q	1406	0	1382	10	0
2	R	1406	0	1382	6	0
2	S	1406	0	1382	10	0
3	A	24	0	0	0	0
3	B	15	0	0	0	0
3	C	140	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	127	0	0	2	0
3	E	121	0	0	0	0
3	F	129	0	0	1	0
3	G	53	0	0	0	0
3	H	135	0	0	2	0
3	I	148	0	0	1	0
3	J	45	0	0	0	0
3	K	45	0	0	1	0
3	L	116	0	0	0	0
3	M	134	0	0	0	0
3	N	118	0	0	1	0
3	O	31	0	0	1	0
3	P	54	0	0	2	0
3	Q	101	0	0	1	0
3	R	111	0	0	0	0
3	S	93	0	0	2	0
3	T	32	0	0	0	0
3	V	23	0	0	0	0
3	X	50	0	0	0	0
3	Y	23	0	0	0	0
3	Z	13	0	0	0	0
All	All	29978	0	27845	251	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 4.

All (251) 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)
2:L:373:ILE:HD11	1:V:70:VAL:HG21	1.30	1.07
2:C:374:ASN:HB3	2:C:440:THR:HG21	1.45	0.98
2:D:440:THR:HG23	3:D:2056:HOH:O	1.64	0.95
1:B:70:VAL:HG21	2:D:373:ILE:HD11	1.46	0.95
2:F:462:LEU:HD21	2:F:542:GLN:HG2	1.47	0.94
2:N:374:ASN:HB3	2:N:440:THR:HG21	1.47	0.94
2:F:440:THR:HG23	3:F:2053:HOH:O	1.67	0.93
1:G:55:ILE:CD1	1:G:122:VAL:HG13	2.07	0.85
1:K:55:ILE:CD1	1:K:122:VAL:HG13	2.08	0.84
1:V:37:ALA:HB2	1:V:110:LEU:HD11	1.60	0.83
2:L:373:ILE:CD1	1:V:70:VAL:HG21	2.09	0.83
2:L:373:ILE:HD11	1:V:70:VAL:CG2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:373:ILE:HD11	1:X:70:VAL:HG21	1.59	0.82
1:A:92:HIS:CE1	1:A:106:ASN:HD21	1.97	0.82
1:G:70:VAL:HG21	2:R:373:ILE:HD11	1.60	0.81
1:G:55:ILE:HD12	1:G:122:VAL:HG13	1.64	0.80
1:X:37:ALA:HB2	1:X:110:LEU:HD11	1.65	0.79
1:T:55:ILE:HD12	1:T:98:LEU:HD21	1.65	0.78
1:Y:37:ALA:HB2	1:Y:110:LEU:HD11	1.67	0.76
1:Y:39:LEU:HD22	1:Y:133:ILE:HG21	1.68	0.75
1:O:55:ILE:HD12	1:O:98:LEU:HD21	1.68	0.75
1:K:55:ILE:HD12	1:K:122:VAL:HG13	1.68	0.74
1:J:37:ALA:HB2	1:J:110:LEU:HD11	1.71	0.73
1:Y:55:ILE:HD12	1:Y:98:LEU:HD21	1.69	0.72
1:O:29:ILE:HD12	1:O:133:ILE:HG21	1.73	0.71
1:X:17:ALA:HB2	1:X:44:THR:HG21	1.76	0.68
1:B:74:TYR:CD1	1:B:98:LEU:HD13	2.29	0.67
1:X:112:LEU:HD21	1:X:139:VAL:HG23	1.77	0.67
2:F:410:ILE:HD13	2:F:527:LEU:HD12	1.76	0.67
1:G:70:VAL:HG21	2:R:373:ILE:CD1	2.25	0.67
1:G:70:VAL:CG2	2:R:373:ILE:HD11	2.25	0.66
1:Y:87:LEU:HD22	1:Y:91:VAL:HG13	1.77	0.66
2:H:527:LEU:HD23	2:H:529:LYS:HE2	1.77	0.66
2:N:440:THR:HG22	3:N:2051:HOH:O	1.94	0.66
1:O:70:VAL:HG11	1:O:73:LEU:HD21	1.78	0.66
1:Y:123:LYS:HG2	1:Y:128:VAL:HG13	1.77	0.65
2:Q:421:ILE:HD13	2:Q:505:LYS:HE2	1.78	0.64
2:M:377:ILE:HD12	2:M:382:VAL:HG21	1.80	0.63
1:B:93:PHE:CE1	1:B:98:LEU:HD11	2.34	0.63
1:J:87:LEU:HD13	1:J:91:VAL:HG21	1.80	0.63
1:V:17:ALA:HB2	1:V:44:THR:HG21	1.81	0.63
1:K:55:ILE:HD11	1:K:122:VAL:HG13	1.78	0.62
2:Q:361:ALA:N	3:Q:2012:HOH:O	2.32	0.61
1:J:91:VAL:HG22	1:J:107:VAL:HG22	1.82	0.61
1:X:33:LYS:HE2	1:X:139:VAL:HG13	1.81	0.61
1:O:58:LEU:HD23	1:O:70:VAL:HA	1.83	0.61
1:G:123:LYS:HG2	1:G:128:VAL:HG13	1.82	0.60
1:Z:37:ALA:HB2	1:Z:110:LEU:HD11	1.82	0.60
1:B:55:ILE:HD13	1:B:122:VAL:HG13	1.83	0.59
1:K:36:THR:HG22	3:K:2003:HOH:O	2.02	0.59
2:H:483:ASP:O	2:H:487:VAL:HG22	2.03	0.59
1:Y:87:LEU:HD13	1:Y:91:VAL:HG11	1.85	0.59
1:J:55:ILE:HD12	1:J:98:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:36:THR:HG22	1:T:108:THR:HA	1.84	0.59
1:B:70:VAL:HG21	2:D:373:ILE:CD1	2.26	0.58
1:P:55:ILE:HD12	1:P:122:VAL:HG22	1.85	0.58
1:T:37:ALA:HB2	1:T:110:LEU:HD11	1.86	0.58
1:B:39:LEU:HD12	1:B:105:ILE:HD11	1.86	0.57
2:M:382:VAL:HG23	2:M:383:ILE:HG12	1.85	0.57
2:S:373:ILE:CD1	1:Z:70:VAL:HG11	2.34	0.57
1:G:58:LEU:HD23	1:G:70:VAL:HA	1.86	0.57
1:Z:29:ILE:HG21	1:Z:31:LYS:HZ1	1.69	0.57
1:J:123:LYS:HG2	1:J:128:VAL:HG13	1.85	0.57
2:C:374:ASN:CB	2:C:440:THR:HG21	2.29	0.56
1:V:55:ILE:O	1:V:73:LEU:HD12	2.05	0.56
1:A:37:ALA:HB2	1:A:110:LEU:HD11	1.86	0.56
2:E:410:ILE:HD13	2:E:527:LEU:HD12	1.87	0.55
1:X:112:LEU:HD11	1:X:139:VAL:CG2	2.37	0.55
1:O:37:ALA:HB2	1:O:110:LEU:HD11	1.89	0.55
1:A:123:LYS:HG2	1:A:128:VAL:HG13	1.88	0.55
2:D:467:ARG:HB3	2:D:467:ARG:CZ	2.38	0.54
2:S:373:ILE:HD12	1:Z:70:VAL:HG11	1.89	0.54
1:X:58:LEU:HD23	1:X:70:VAL:HA	1.89	0.54
1:T:55:ILE:CD1	1:T:98:LEU:HD21	2.36	0.54
1:O:87:LEU:HB3	1:O:91:VAL:HG23	1.90	0.53
1:P:106:ASN:C	1:P:106:ASN:HD22	2.13	0.53
1:B:54:ASP:HB3	1:B:123:LYS:HB2	1.90	0.53
2:H:503:LYS:NZ	3:H:2105:HOH:O	2.31	0.52
1:B:36:THR:HG23	1:B:107:VAL:O	2.10	0.52
2:C:373:ILE:HD11	1:T:70:VAL:HG21	1.91	0.52
2:R:437:ASN:O	2:R:440:THR:HG22	2.10	0.52
1:Z:36:THR:HG23	1:Z:108:THR:HG22	1.92	0.52
2:C:483:ASP:O	2:C:487:VAL:HG22	2.09	0.52
2:S:374:ASN:CB	2:S:440:THR:HG21	2.39	0.52
1:T:59:ILE:HG23	1:T:61:PRO:HD3	1.92	0.52
1:V:87:LEU:HD23	1:V:90:ARG:NH2	2.24	0.52
1:B:55:ILE:CD1	1:B:122:VAL:HG13	2.40	0.52
1:Y:55:ILE:CD1	1:Y:98:LEU:HD21	2.38	0.52
1:B:20:LEU:HD13	1:B:45:LEU:HD23	1.91	0.51
1:G:55:ILE:HD11	1:G:122:VAL:HG13	1.90	0.51
1:O:29:ILE:HD12	1:O:133:ILE:CG2	2.41	0.51
2:L:483:ASP:O	2:L:487:VAL:HG22	2.11	0.51
1:O:55:ILE:HD13	1:O:103:ALA:HB2	1.93	0.51
1:Z:93:PHE:CD1	1:Z:98:LEU:HD21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:410:ILE:CD1	2:F:527:LEU:HD12	2.41	0.51
2:D:483:ASP:O	2:D:487:VAL:HG22	2.11	0.51
2:E:373:ILE:HD11	1:O:70:VAL:HG21	1.92	0.51
2:N:374:ASN:CB	2:N:440:THR:HG21	2.30	0.51
1:X:93:PHE:CG	1:X:98:LEU:HD21	2.46	0.51
1:O:123:LYS:HG2	1:O:128:VAL:HG13	1.93	0.50
2:D:422:MET:HG2	2:D:436:ILE:HB	1.92	0.50
2:I:395:LEU:HD23	2:I:538:VAL:HA	1.94	0.50
2:L:437:ASN:O	2:L:440:THR:HG22	2.12	0.50
2:N:373:ILE:HD11	1:Y:70:VAL:HG21	1.94	0.49
1:P:96:ASN:OD1	1:P:97:ASP:N	2.45	0.49
1:G:22:ILE:HD11	1:G:122:VAL:HG23	1.95	0.49
1:Y:98:LEU:C	1:Y:98:LEU:HD23	2.33	0.49
2:I:373:ILE:HD12	1:P:70:VAL:HG11	1.95	0.49
1:G:64:ASN:HD21	1:G:66:LYS:NZ	2.10	0.49
1:X:112:LEU:HD11	1:X:139:VAL:HG21	1.95	0.49
1:K:53:LEU:HD11	1:K:55:ILE:HD11	1.96	0.48
2:M:483:ASP:O	2:M:487:VAL:HG22	2.13	0.48
2:C:417:GLN:NE2	3:C:2050:HOH:O	2.40	0.48
2:C:477:ILE:HG22	2:H:531:ASP:OD2	2.13	0.48
1:O:54:ASP:HB3	1:O:123:LYS:HB2	1.94	0.48
1:A:55:ILE:CD1	1:A:122:VAL:HG13	2.43	0.48
1:G:54:ASP:HB3	1:G:123:LYS:HB2	1.95	0.48
1:Y:54:ASP:HB3	1:Y:123:LYS:HB2	1.96	0.48
2:I:373:ILE:HB	1:P:73:LEU:HD11	1.95	0.48
1:K:123:LYS:HG2	1:K:128:VAL:HG13	1.95	0.48
2:E:395:LEU:HD23	2:E:538:VAL:HA	1.96	0.48
1:A:70:VAL:HG21	2:Q:373:ILE:HD11	1.94	0.48
2:S:440:THR:HG23	3:S:2007:HOH:O	2.14	0.48
1:Z:55:ILE:HD13	1:Z:103:ALA:HB2	1.96	0.48
1:B:72:ILE:HG21	1:B:105:ILE:HG21	1.96	0.47
1:A:84:TYR:CD2	1:A:87:LEU:HD12	2.50	0.47
1:K:123:LYS:HG2	1:K:128:VAL:CG1	2.45	0.47
2:S:398:VAL:O	2:S:534:THR:HA	2.15	0.47
2:H:422:MET:HG2	2:H:436:ILE:HB	1.97	0.47
1:V:33:LYS:NZ	1:V:111:GLN:OE1	2.48	0.47
1:X:94:THR:HG22	1:X:106:ASN:ND2	2.30	0.47
2:C:440:THR:HB	3:C:2066:HOH:O	2.15	0.47
1:B:55:ILE:HD12	1:B:122:VAL:HG22	1.96	0.46
1:X:123:LYS:HG2	1:X:128:VAL:HG13	1.97	0.46
1:G:37:ALA:HB2	1:G:110:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:74:TYR:CZ	1:T:77:ASP:HA	2.49	0.46
1:Z:43:PHE:CZ	1:Z:101:GLY:HA2	2.51	0.46
1:A:56:GLU:CB	1:A:73:LEU:HD23	2.45	0.46
1:T:28:MET:HG2	1:T:134:HIS:HB2	1.97	0.46
2:H:369:PRO:HA	3:H:2023:HOH:O	2.16	0.46
1:K:37:ALA:HB2	1:K:110:LEU:HD11	1.96	0.46
1:P:55:ILE:HB	1:P:74:TYR:HB3	1.97	0.46
2:Q:531:ASP:OD2	2:S:477:ILE:HG22	2.15	0.46
1:B:92:HIS:HB2	1:B:106:ASN:HD21	1.81	0.46
2:E:423:GLU:HB3	2:E:508:ALA:HB2	1.98	0.45
1:A:70:VAL:HG21	2:Q:373:ILE:CD1	2.46	0.45
2:Q:483:ASP:O	2:Q:487:VAL:HG22	2.17	0.45
1:O:87:LEU:HD13	1:O:91:VAL:HG21	1.98	0.45
1:P:73:LEU:CD2	3:P:2014:HOH:O	2.65	0.45
2:Q:477:ILE:HG22	2:R:531:ASP:OD2	2.15	0.45
1:K:31:LYS:NZ	1:K:36:THR:O	2.49	0.45
1:X:17:ALA:HB2	1:X:44:THR:CG2	2.45	0.45
2:S:411:VAL:HG13	2:S:528:PHE:HB2	1.99	0.45
1:P:98:LEU:C	1:P:98:LEU:HD23	2.37	0.45
2:D:361:ALA:N	3:D:2011:HOH:O	2.49	0.45
1:J:73:LEU:C	1:J:73:LEU:HD12	2.37	0.45
1:K:59:ILE:HD13	1:K:118:TYR:CE2	2.52	0.45
1:B:131:LYS:HE2	1:B:133:ILE:HD11	1.99	0.45
2:E:384:ARG:NH2	1:O:70:VAL:HG23	2.31	0.45
1:G:39:LEU:HD12	1:G:105:ILE:HD11	1.99	0.45
2:D:366:TRP:CE2	2:D:368:GLY:HA2	2.52	0.44
2:D:374:ASN:HB3	2:D:440:THR:HG21	1.99	0.44
1:P:73:LEU:HD22	3:P:2014:HOH:O	2.17	0.44
1:G:58:LEU:HD13	1:G:68:ASP:HB3	1.99	0.44
1:B:56:GLU:HB2	1:B:73:LEU:HD23	1.99	0.44
1:V:55:ILE:HB	1:V:74:TYR:HB3	1.99	0.44
1:T:87:LEU:HB3	1:T:91:VAL:HG23	2.00	0.44
1:Y:39:LEU:HD21	1:Y:135:LEU:HD13	2.00	0.44
1:B:20:LEU:HD21	1:B:122:VAL:HG12	2.00	0.44
2:E:373:ILE:HD12	1:O:73:LEU:HD11	2.00	0.44
1:V:38:TYR:CE1	1:V:94:THR:HG21	2.53	0.44
1:V:55:ILE:HD13	1:V:103:ALA:HB2	2.00	0.44
1:Y:20:LEU:HD23	1:Y:21:SER:N	2.33	0.44
1:Z:46:SER:OG	1:Z:47:PRO:HD2	2.17	0.44
1:B:98:LEU:HD23	1:B:98:LEU:O	2.18	0.43
2:E:384:ARG:NH2	1:O:70:VAL:CG2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:ILE:CD1	2:E:527:LEU:HD12	2.48	0.43
2:R:421:ILE:HG12	2:R:513:THR:HG23	2.00	0.43
1:V:54:ASP:HB3	1:V:123:LYS:HB2	2.01	0.43
2:Q:422:MET:HG2	2:Q:436:ILE:HB	2.00	0.43
1:J:46:SER:HB2	1:J:47:PRO:HD2	2.00	0.43
1:Z:119:GLN:HE21	1:Z:130:ASN:ND2	2.17	0.43
2:H:441:THR:HG23	1:J:125:ALA:HB2	2.01	0.43
1:T:29:ILE:HD13	1:T:133:ILE:HG21	2.01	0.43
1:O:55:ILE:CD1	1:O:98:LEU:HD21	2.42	0.43
1:P:54:ASP:HB3	1:P:123:LYS:HB2	2.00	0.43
2:F:386:PHE:O	2:F:400:ALA:HA	2.19	0.43
2:Q:366:TRP:CE2	2:Q:368:GLY:HA2	2.54	0.42
2:M:417:GLN:CD	2:M:517:LEU:HD23	2.40	0.42
2:I:373:ILE:CD1	1:P:70:VAL:HG21	2.49	0.42
2:I:423:GLU:OE2	2:I:505:LYS:HG2	2.19	0.42
1:K:73:LEU:HD12	1:K:73:LEU:C	2.40	0.42
1:O:56:GLU:OE1	3:O:2009:HOH:O	2.21	0.42
1:B:57:TRP:HB2	1:B:72:ILE:HG22	2.02	0.42
2:L:422:MET:HG2	2:L:436:ILE:HB	2.01	0.42
1:P:37:ALA:HB2	1:P:110:LEU:HD11	2.00	0.42
1:A:73:LEU:HD12	1:A:83:TYR:OH	2.20	0.42
3:I:2018:HOH:O	1:P:73:LEU:HD21	2.19	0.42
1:K:119:GLN:HA	1:K:131:LYS:O	2.19	0.42
1:O:32:ALA:HB3	1:O:35:GLU:HG3	2.02	0.42
1:P:73:LEU:HD12	1:P:83:TYR:OH	2.19	0.42
1:A:58:LEU:HD23	1:A:70:VAL:HA	2.01	0.42
1:J:55:ILE:HD12	1:J:98:LEU:CD2	2.48	0.42
1:O:131:LYS:HE2	1:O:133:ILE:HD11	2.00	0.42
1:Z:123:LYS:HG2	1:Z:128:VAL:HG13	2.01	0.42
1:A:55:ILE:HD12	1:A:122:VAL:HG22	2.01	0.42
1:A:92:HIS:CE1	1:A:106:ASN:ND2	2.77	0.42
2:L:421:ILE:HD13	2:L:505:LYS:HD3	2.02	0.42
1:Y:53:LEU:CD2	1:Y:99:LYS:HA	2.50	0.42
1:K:70:VAL:HG13	1:K:83:TYR:HB3	2.01	0.41
1:Y:121:LYS:HG2	1:Y:130:ASN:HB3	2.02	0.41
1:B:53:LEU:HD11	1:B:55:ILE:HD11	2.02	0.41
2:E:404:GLY:HA3	2:E:408:TYR:O	2.19	0.41
2:F:542:GLN:HA	2:F:542:GLN:HE21	1.85	0.41
1:O:70:VAL:CG1	1:O:73:LEU:HD21	2.49	0.41
2:C:373:ILE:HD12	1:T:70:VAL:HG11	2.01	0.41
2:D:398:VAL:O	2:D:534:THR:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:121:LYS:HG2	1:T:130:ASN:HB3	2.03	0.41
2:L:531:ASP:OD2	2:N:477:ILE:HG22	2.21	0.41
1:Y:87:LEU:HD13	1:Y:91:VAL:CG1	2.51	0.41
2:F:413:PRO:HB2	2:M:378:ASN:O	2.20	0.41
1:X:39:LEU:HB3	1:X:133:ILE:HD12	2.02	0.41
2:N:487:VAL:HG11	2:N:493:ARG:HD2	2.03	0.41
2:S:422:MET:HG2	2:S:436:ILE:HB	2.02	0.41
2:S:440:THR:CG2	3:S:2007:HOH:O	2.69	0.41
1:Z:31:LYS:HZ3	1:Z:37:ALA:HB1	1.85	0.41
2:F:361:ALA:HB1	2:F:362:PRO:HD2	2.03	0.41
2:I:483:ASP:O	2:I:487:VAL:HG22	2.21	0.41
1:J:112:LEU:HD11	1:J:139:VAL:CG2	2.50	0.41
1:T:54:ASP:HB3	1:T:123:LYS:HB2	2.03	0.41
1:V:17:ALA:HB2	1:V:44:THR:CG2	2.51	0.41
1:Y:131:LYS:HE2	1:Y:133:ILE:HD11	2.01	0.41
2:N:410:ILE:HD13	2:N:527:LEU:HA	2.02	0.41
1:T:87:LEU:HD23	1:T:90:ARG:NH2	2.35	0.41
1:G:56:GLU:HB2	1:G:73:LEU:HD23	2.01	0.40
2:L:417:GLN:HG2	2:L:517:LEU:HA	2.02	0.40
2:N:373:ILE:HG22	2:N:381:PRO:HB2	2.04	0.40
1:A:26:GLU:HA	1:A:132:LYS:O	2.21	0.40
1:B:96:ASN:OD1	1:B:96:ASN:N	2.44	0.40
2:L:363:ILE:HG12	2:L:364:THR:N	2.36	0.40
1:B:31:LYS:HG3	1:B:37:ALA:HB2	2.04	0.40
2:S:373:ILE:HD11	1:Z:70:VAL:HG11	2.01	0.40
2:C:373:ILE:CD1	1:T:70:VAL:HG21	2.51	0.40
2:N:373:ILE:CD1	1:Y:70:VAL:HG21	2.50	0.40
2:N:495:ILE:HG22	2:N:519:PHE:HA	2.04	0.40
1:B:45:LEU:HD13	1:B:124:LYS:HD3	2.02	0.40
2:H:366:TRP:CE2	2:H:368:GLY:HA2	2.56	0.40
1:O:55:ILE:HB	1:O:74:TYR:HB3	2.04	0.40
2:Q:391:ARG:HG2	2:Q:462:LEU:HB3	2.03	0.40
1:T:29:ILE:HD13	1:T:133:ILE:CG2	2.52	0.40
1:V:20:LEU:HD23	1:V:20:LEU:C	2.42	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	115/128 (90%)	107 (93%)	7 (6%)	1 (1%)	17	20
1	B	107/128 (84%)	96 (90%)	11 (10%)	0	100	100
1	G	121/128 (94%)	115 (95%)	6 (5%)	0	100	100
1	J	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
1	K	121/128 (94%)	116 (96%)	5 (4%)	0	100	100
1	O	114/128 (89%)	107 (94%)	7 (6%)	0	100	100
1	P	121/128 (94%)	115 (95%)	6 (5%)	0	100	100
1	T	117/128 (91%)	109 (93%)	8 (7%)	0	100	100
1	V	119/128 (93%)	114 (96%)	5 (4%)	0	100	100
1	X	121/128 (94%)	117 (97%)	4 (3%)	0	100	100
1	Y	117/128 (91%)	109 (93%)	8 (7%)	0	100	100
1	Z	115/128 (90%)	106 (92%)	8 (7%)	1 (1%)	17	20
2	C	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	D	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	E	180/197 (91%)	172 (96%)	8 (4%)	0	100	100
2	F	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	H	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	I	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	L	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	M	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	N	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	Q	180/197 (91%)	174 (97%)	6 (3%)	0	100	100
2	R	180/197 (91%)	173 (96%)	7 (4%)	0	100	100
2	S	180/197 (91%)	171 (95%)	9 (5%)	0	100	100
All	All	3569/3900 (92%)	3408 (96%)	159 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	101	GLY
1	A	24	THR

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	104/113 (92%)	98 (94%)	6 (6%)	20	27
1	B	99/113 (88%)	94 (95%)	5 (5%)	24	33
1	G	109/113 (96%)	104 (95%)	5 (5%)	27	38
1	J	109/113 (96%)	105 (96%)	4 (4%)	34	48
1	K	109/113 (96%)	106 (97%)	3 (3%)	43	60
1	O	105/113 (93%)	100 (95%)	5 (5%)	25	36
1	P	109/113 (96%)	106 (97%)	3 (3%)	43	60
1	T	106/113 (94%)	102 (96%)	4 (4%)	33	47
1	V	107/113 (95%)	103 (96%)	4 (4%)	34	48
1	X	109/113 (96%)	104 (95%)	5 (5%)	27	38
1	Y	106/113 (94%)	100 (94%)	6 (6%)	20	28
1	Z	104/113 (92%)	99 (95%)	5 (5%)	25	36
2	C	159/171 (93%)	153 (96%)	6 (4%)	33	47
2	D	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	E	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	F	159/171 (93%)	154 (97%)	5 (3%)	40	55
2	H	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	I	159/171 (93%)	155 (98%)	4 (2%)	47	65
2	L	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	M	159/171 (93%)	154 (97%)	5 (3%)	40	55
2	N	159/171 (93%)	154 (97%)	5 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	159/171 (93%)	155 (98%)	4 (2%)	47	65
2	R	159/171 (93%)	156 (98%)	3 (2%)	57	73
2	S	159/171 (93%)	155 (98%)	4 (2%)	47	65
All	All	3184/3408 (93%)	3081 (97%)	103 (3%)	39	54

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	MET
1	A	42	LYS
1	A	70	VAL
1	A	99	LYS
1	A	106	ASN
1	A	128	VAL
1	B	48	GLU
1	B	77	ASP
1	B	106	ASN
1	B	114	ASP
1	B	135	LEU
2	C	363	ILE
2	C	366	TRP
2	C	372	SER
2	C	426	GLN
2	C	440	THR
2	C	455	ARG
2	D	363	ILE
2	D	366	TRP
2	D	521	ARG
2	E	366	TRP
2	E	372	SER
2	E	417	GLN
2	F	363	ILE
2	F	366	TRP
2	F	440	THR
2	F	507	VAL
2	F	542	GLN
1	G	18	ARG
1	G	36	THR
1	G	67	VAL
1	G	70	VAL
1	G	128	VAL

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Mol	Chain	Res	Type
2	H	363	ILE
2	H	366	TRP
2	H	417	GLN
2	I	363	ILE
2	I	366	TRP
2	I	379	ASP
2	I	503	LYS
1	J	33	LYS
1	J	59	ILE
1	J	73	LEU
1	J	100	SER
1	K	113	SER
1	K	128	VAL
1	K	130	ASN
2	L	363	ILE
2	L	366	TRP
2	L	372	SER
2	M	363	ILE
2	M	366	TRP
2	M	372	SER
2	M	416	SER
2	M	455	ARG
2	N	363	ILE
2	N	366	TRP
2	N	372	SER
2	N	455	ARG
2	N	529	LYS
1	O	33	LYS
1	O	96	ASN
1	O	99	LYS
1	O	111	GLN
1	O	128	VAL
1	P	70	VAL
1	P	92	HIS
1	P	106	ASN
2	Q	363	ILE
2	Q	366	TRP
2	Q	372	SER
2	Q	521	ARG
2	R	363	ILE
2	R	366	TRP
2	R	455	ARG

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Mol	Chain	Res	Type
2	S	363	ILE
2	S	366	TRP
2	S	372	SER
2	S	455	ARG
1	T	28	MET
1	T	59	ILE
1	T	70	VAL
1	T	130	ASN
1	V	28	MET
1	V	42	LYS
1	V	70	VAL
1	V	106	ASN
1	X	23	THR
1	X	26	GLU
1	X	64	ASN
1	X	70	VAL
1	X	96	ASN
1	Y	70	VAL
1	Y	73	LEU
1	Y	77	ASP
1	Y	100	SER
1	Y	128	VAL
1	Y	130	ASN
1	Z	48	GLU
1	Z	70	VAL
1	Z	91	VAL
1	Z	99	LYS
1	Z	106	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	134	HIS
1	B	106	ASN
2	F	542	GLN
1	G	64	ASN
1	G	134	HIS
1	P	106	ASN
2	S	378	ASN
2	S	458	HIS
2	S	542	GLN

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Mol	Chain	Res	Type
1	T	130	ASN
1	V	106	ASN
1	X	64	ASN
1	X	134	HIS
1	Y	109	ASN
1	Y	111	GLN
1	Z	130	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	117/128 (91%)	1.39	36 (30%)	0	0	34, 44, 54, 57	0
1	B	113/128 (88%)	1.95	47 (41%)	0	0	32, 46, 58, 60	0
1	G	123/128 (96%)	0.08	6 (4%)	29	36	33, 44, 55, 58	0
1	J	123/128 (96%)	0.18	7 (5%)	23	30	33, 44, 55, 57	0
1	K	123/128 (96%)	0.27	5 (4%)	37	44	33, 45, 56, 57	0
1	O	118/128 (92%)	0.21	4 (3%)	45	52	33, 44, 54, 58	0
1	P	123/128 (96%)	0.47	12 (9%)	7	10	33, 44, 55, 57	0
1	T	119/128 (92%)	0.64	11 (9%)	9	12	33, 45, 55, 57	0
1	V	121/128 (94%)	1.16	29 (23%)	0	0	34, 44, 55, 57	0
1	X	123/128 (96%)	0.25	9 (7%)	15	20	33, 45, 55, 58	0
1	Y	119/128 (92%)	0.99	24 (20%)	1	1	34, 44, 54, 57	0
1	Z	117/128 (91%)	1.59	43 (36%)	0	0	34, 45, 55, 57	0
2	C	182/197 (92%)	-0.05	0	100	100	19, 24, 30, 36	0
2	D	182/197 (92%)	0.26	5 (2%)	54	62	20, 25, 33, 36	0
2	E	182/197 (92%)	-0.00	1 (0%)	91	94	20, 25, 32, 36	0
2	F	182/197 (92%)	-0.01	0	100	100	19, 23, 30, 34	0
2	H	182/197 (92%)	-0.17	0	100	100	19, 24, 30, 35	0
2	I	182/197 (92%)	0.09	0	100	100	19, 25, 30, 35	0
2	L	182/197 (92%)	0.18	3 (1%)	72	77	22, 27, 34, 36	0
2	M	182/197 (92%)	0.10	3 (1%)	72	77	21, 25, 30, 33	0
2	N	182/197 (92%)	-0.04	0	100	100	21, 26, 32, 37	0
2	Q	182/197 (92%)	0.37	12 (6%)	18	23	22, 29, 34, 39	0
2	R	182/197 (92%)	-0.03	0	100	100	22, 27, 34, 39	0
2	S	182/197 (92%)	-0.09	0	100	100	24, 31, 39, 41	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3623/3900 (92%)	0.33	257 (7%)	16	21	19, 30, 52, 60	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ALA	8.6
1	Y	112	LEU	6.6
1	V	34	GLY	6.4
1	B	91	VAL	6.0
1	B	136	VAL	6.0
1	Z	112	LEU	5.7
1	B	138	LEU	5.6
1	A	107	VAL	5.4
1	Z	25	PRO	5.4
1	Y	115	ILE	5.2
1	B	137	VAL	5.2
1	Z	107	VAL	5.2
1	Z	31	LYS	5.0
1	B	39	LEU	4.9
1	B	107	VAL	4.9
1	B	37	ALA	4.9
1	V	108	THR	4.8
1	Y	137	VAL	4.8
1	V	107	VAL	4.7
1	T	112	LEU	4.7
1	B	25	PRO	4.7
1	V	82	ASP	4.6
1	A	25	PRO	4.6
1	B	115	ILE	4.5
1	B	24	THR	4.5
1	B	18	ARG	4.5
1	Z	113	SER	4.4
1	B	105	ILE	4.4
1	Z	24	THR	4.4
1	V	33	LYS	4.3
1	V	109	ASN	4.3
1	T	25	PRO	4.3
1	V	87	LEU	4.2
1	A	32	ALA	4.2
1	V	37	ALA	4.2
1	B	83	TYR	4.2
1	P	25	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	85	PRO	4.1
1	Z	98	LEU	4.1
1	X	25	PRO	4.0
1	V	89	GLY	4.0
1	A	39	LEU	3.9
1	Z	110	LEU	3.9
1	B	28	MET	3.9
1	B	30	GLU	3.9
1	V	110	LEU	3.9
1	A	91	VAL	3.9
1	Z	91	VAL	3.9
1	V	92	HIS	3.9
1	B	84	TYR	3.8
1	T	136	VAL	3.8
1	V	85	PRO	3.8
1	A	36	THR	3.8
1	Z	36	THR	3.8
1	Z	135	LEU	3.8
1	A	64	ASN	3.8
1	A	65	GLN	3.8
1	B	61	PRO	3.8
1	Z	64	ASN	3.7
1	Z	23	THR	3.7
1	V	137	VAL	3.7
1	X	82	ASP	3.7
1	B	106	ASN	3.6
1	Y	37	ALA	3.5
1	B	27	GLU	3.5
1	B	133	ILE	3.5
1	A	37	ALA	3.5
1	B	114	ASP	3.5
1	V	112	LEU	3.5
1	Y	135	LEU	3.5
1	P	82	ASP	3.5
1	Z	32	ALA	3.5
1	B	17	ALA	3.5
1	A	85	PRO	3.4
1	V	135	LEU	3.4
1	T	82	ASP	3.4
1	V	28	MET	3.4
1	A	112	LEU	3.4
1	Y	64	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	Y	32	ALA	3.3
1	Z	37	ALA	3.3
1	B	135	LEU	3.3
2	Q	398	VAL	3.3
1	B	117	THR	3.3
1	J	24	THR	3.3
1	B	62	ALA	3.3
1	A	92	HIS	3.3
1	Z	30	GLU	3.3
1	B	41	CYS	3.3
1	Y	28	MET	3.3
1	X	138	LEU	3.2
1	B	92	HIS	3.2
1	Z	35	GLU	3.2
1	Y	29	ILE	3.2
1	B	86	ASP	3.2
1	Y	113	SER	3.2
1	V	111	GLN	3.2
1	Z	115	ILE	3.2
1	B	94	THR	3.2
1	P	96	ASN	3.2
1	Y	136	VAL	3.2
1	Z	96	ASN	3.2
1	B	82	ASP	3.2
1	Z	93	PHE	3.2
1	A	33	LYS	3.2
1	A	105	ILE	3.1
1	V	35	GLU	3.1
1	K	16	PHE	3.1
1	Z	28	MET	3.1
1	B	96	ASN	3.1
1	J	17	ALA	3.1
1	Z	57	TRP	3.1
1	B	72	ILE	3.1
1	Y	30	GLU	3.1
1	V	96	ASN	3.1
1	Z	62	ALA	3.1
1	P	139	VAL	3.1
1	Y	39	LEU	3.1
1	Y	110	LEU	3.0
1	A	31	LYS	3.0
1	X	112	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	18	ARG	2.9
1	K	25	PRO	2.9
1	A	84	TYR	2.9
1	B	38	TYR	2.9
1	V	84	TYR	2.9
1	A	59	ILE	2.9
1	B	103	ALA	2.9
1	Y	25	PRO	2.9
1	K	138	LEU	2.9
1	P	92	HIS	2.9
1	Z	94	THR	2.8
1	V	91	VAL	2.8
1	V	25	PRO	2.8
1	Z	106	ASN	2.8
2	Q	499	LEU	2.8
1	T	113	SER	2.8
1	B	131	LYS	2.8
1	Z	61	PRO	2.7
1	O	139	VAL	2.7
2	D	398	VAL	2.7
1	Z	39	LEU	2.7
1	Y	33	LYS	2.7
1	Y	107	VAL	2.7
1	K	65	GLN	2.7
1	Z	42	LYS	2.7
1	Z	118	TYR	2.7
1	J	138	LEU	2.7
1	B	89	GLY	2.7
1	Z	89	GLY	2.7
1	B	87	LEU	2.7
1	Z	82	ASP	2.7
1	B	70	VAL	2.7
2	Q	389	LEU	2.7
1	A	63	ASP	2.6
1	O	96	ASN	2.6
1	P	89	GLY	2.6
1	Z	116	GLY	2.6
1	B	118	TYR	2.6
1	Y	105	ILE	2.6
1	P	107	VAL	2.6
1	Z	38	TYR	2.6
1	X	18	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	T	111	GLN	2.6
1	A	19	SER	2.6
1	A	96	ASN	2.6
1	X	64	ASN	2.6
1	Y	111	GLN	2.6
1	A	108	THR	2.6
1	B	36	THR	2.5
1	A	116	GLY	2.5
1	T	63	ASP	2.5
1	Y	109	ASN	2.5
2	Q	512	LEU	2.5
1	P	109	ASN	2.5
1	V	88	LYS	2.5
1	A	82	ASP	2.5
1	G	25	PRO	2.5
1	T	87	LEU	2.5
1	V	136	VAL	2.5
1	Z	40	PRO	2.5
1	A	106	ASN	2.5
1	Z	87	LEU	2.5
1	G	28	MET	2.4
1	Z	33	LYS	2.4
1	P	106	ASN	2.4
1	Y	87	LEU	2.4
1	A	133	ILE	2.4
1	A	35	GLU	2.4
1	G	112	LEU	2.4
1	A	93	PHE	2.4
2	D	396	VAL	2.4
1	Z	59	ILE	2.4
1	V	32	ALA	2.4
1	T	108	THR	2.4
2	D	389	LEU	2.3
1	G	65	GLN	2.3
1	A	109	ASN	2.3
1	J	18	ARG	2.3
1	V	90	ARG	2.3
1	Z	26	GLU	2.3
1	V	93	PHE	2.3
2	M	535	PHE	2.3
1	B	88	LYS	2.3
1	O	19	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	Z	109	ASN	2.3
1	B	31	LYS	2.3
1	Z	111	GLN	2.3
1	P	18	ARG	2.2
1	P	32	ALA	2.2
2	D	388	CYS	2.2
1	J	19	SER	2.2
1	Y	34	GLY	2.2
2	Q	537	TYR	2.2
1	V	86	ASP	2.2
1	Z	34	GLY	2.2
2	M	499	LEU	2.2
1	A	89	GLY	2.2
1	J	139	VAL	2.2
1	A	24	THR	2.2
2	D	536	THR	2.2
2	Q	536	THR	2.2
1	G	138	LEU	2.2
1	K	28	MET	2.2
1	Y	85	PRO	2.2
1	Z	19	SER	2.2
1	A	118	TYR	2.1
2	Q	396	VAL	2.1
2	E	400	ALA	2.1
1	B	59	ILE	2.1
1	A	97	ASP	2.1
1	O	62	ALA	2.1
1	X	24	THR	2.1
1	Z	63	ASP	2.1
1	V	65	GLN	2.1
2	Q	469	VAL	2.1
2	Q	535	PHE	2.1
1	T	89	GLY	2.1
1	P	17	ALA	2.1
1	A	48	GLU	2.1
1	X	30	GLU	2.1
2	Q	463	CYS	2.1
1	Y	63	ASP	2.1
2	L	379	ASP	2.1
1	T	97	ASP	2.0
2	M	533	LEU	2.0
1	A	117	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	396	VAL	2.0
2	L	536	THR	2.0
2	Q	534	THR	2.0
1	J	25	PRO	2.0
1	B	29	ILE	2.0
1	B	79	ILE	2.0
2	Q	533	LEU	2.0
1	A	111	GLN	2.0
1	A	94	THR	2.0
1	X	17	ALA	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.