Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:32 PM GMT

PDB ID	:	4P6Z
Title	:	Crystal structure of the human BST2 cytoplasmic domain and the HIV-1 Vpu cytoplasmic domain bound to the clathrin adaptor protein complex 1 (AP1) core
Authors	:	Jia, X.; Xiong, Y.
Deposited on	:	2014-03-25
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:

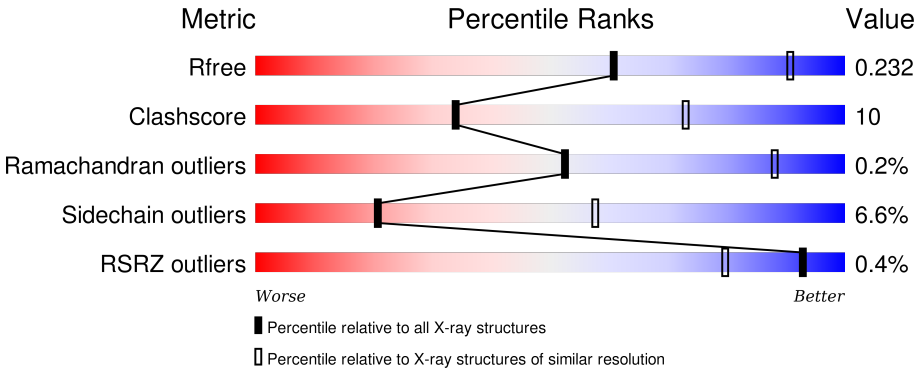
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	G	627	61% 30% • 6%
2	S	158	70% 20% • 7%
3	M	423	76% 21% • •
4	B	600	% 66% 26% • 5%
5	V	63	11% 5% 84%

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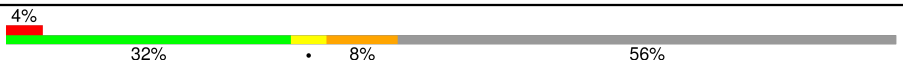
Mol	Chain	Length	Quality of chain
6	T	25	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13940 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 AP-1 complex subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	587	4645	2922	817	867	39	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	MET	-	initiating methionine	UNP P22892
G	-12	GLY	-	expression tag	UNP P22892
G	-11	SER	-	expression tag	UNP P22892
G	-10	SER	-	expression tag	UNP P22892
G	-9	HIS	-	expression tag	UNP P22892
G	-8	HIS	-	expression tag	UNP P22892
G	-7	HIS	-	expression tag	UNP P22892
G	-6	HIS	-	expression tag	UNP P22892
G	-5	HIS	-	expression tag	UNP P22892
G	-4	HIS	-	expression tag	UNP P22892
G	-3	SER	-	expression tag	UNP P22892
G	-2	GLN	-	expression tag	UNP P22892
G	-1	ASP	-	expression tag	UNP P22892
G	0	PRO	-	expression tag	UNP P22892

- Molecule 2 is a protein called AP-1 complex subunit sigma-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	147	1231	796	203	221	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	11	ARG	GLN	engineered mutation	UNP P61966

- Molecule 3 is a protein called AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	415	Total	C	N	O	S	0	1	0
			3370	2166	569	621	14			

- Molecule 4 is a protein called AP-1 complex subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	570	Total	C	N	O	S	0	0	0
			4509	2882	739	861	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP Q10567
B	-14	GLY	-	expression tag	UNP Q10567
B	-13	SER	-	expression tag	UNP Q10567
B	-12	SER	-	expression tag	UNP Q10567
B	-11	HIS	-	expression tag	UNP Q10567
B	-10	HIS	-	expression tag	UNP Q10567
B	-9	HIS	-	expression tag	UNP Q10567
B	-8	HIS	-	expression tag	UNP Q10567
B	-7	HIS	-	expression tag	UNP Q10567
B	-6	HIS	-	expression tag	UNP Q10567
B	-5	SER	-	expression tag	UNP Q10567
B	-4	GLN	-	expression tag	UNP Q10567
B	-3	ASP	-	expression tag	UNP Q10567
B	-2	PRO	-	expression tag	UNP Q10567
B	-1	ASN	-	expression tag	UNP Q10567
B	0	SER	-	expression tag	UNP Q10567
B	431	ALA	THR	engineered mutation	UNP Q10567
B	476	LYS	GLU	engineered mutation	UNP Q10567

- Molecule 5 is a protein called Protein Vpu.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	V	10	Total	C	N	O	0	0	0
			78	47	11	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	18	GLY	-	expression tag	UNP P19554

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Chain	Residue	Modelled	Actual	Comment	Reference
V	19	SER	-	expression tag	UNP P19554
V	20	ASP	-	expression tag	UNP P19554
V	21	GLU	-	expression tag	UNP P19554
V	22	ALA	-	expression tag	UNP P19554
V	23	SER	-	expression tag	UNP P19554
V	24	GLU	-	expression tag	UNP P19554
V	25	GLY	-	expression tag	UNP P19554
V	26	SER	-	expression tag	UNP P19554
V	27	GLY	-	expression tag	UNP P19554

- Molecule 6 is a protein called Bone marrow stromal antigen 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	11	Total	C	N	O	S	0	0	0
			93	58	14	19	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-3	ALA	-	expression tag	UNP Q10589
T	-2	GLY	-	expression tag	UNP Q10589
T	-1	PHE	-	expression tag	UNP Q10589
T	0	SER	-	expression tag	UNP Q10589

- Molecule 7 is water.

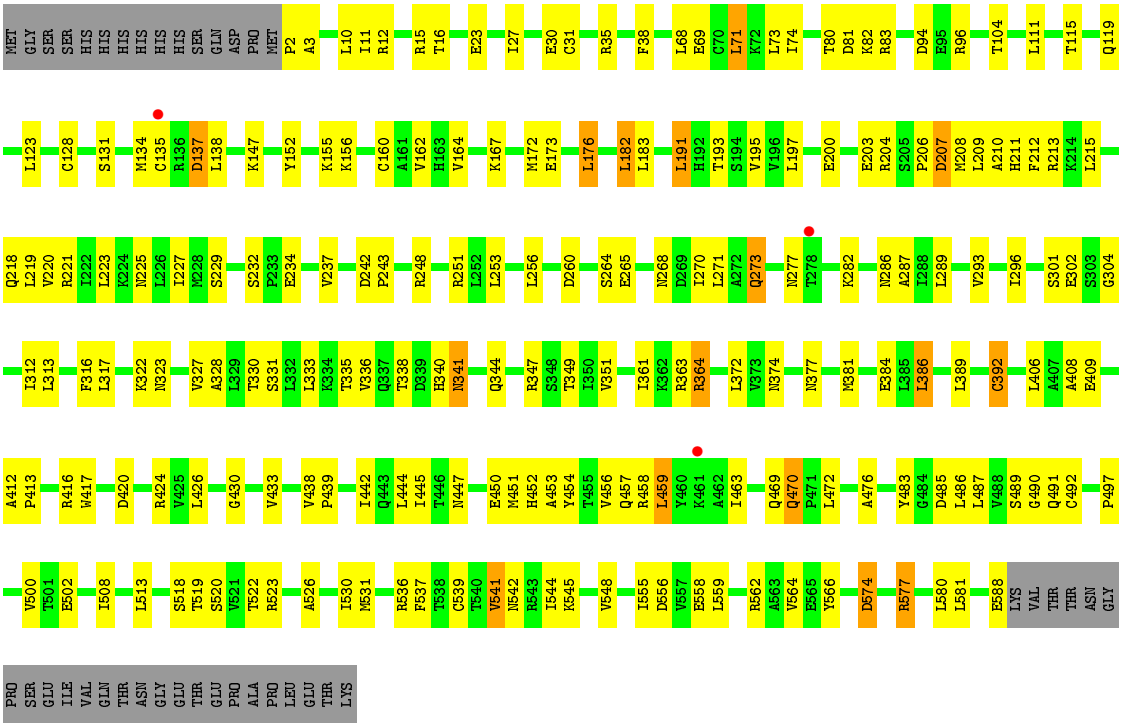
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	4	Total	O	0	0
			4	4		
7	S	3	Total	O	0	0
			3	3		
7	M	5	Total	O	0	0
			5	5		
7	B	2	Total	O	0	0
			2	2		

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.

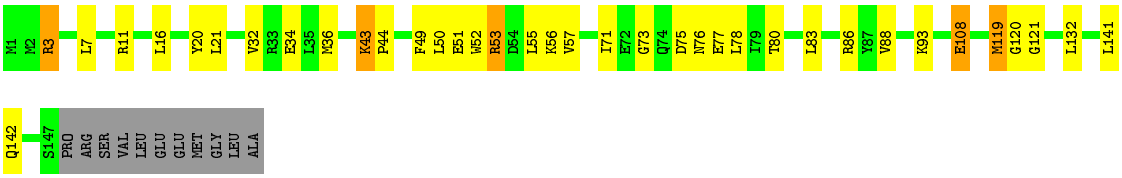
- Molecule 1: AP-1 complex subunit gamma-1

Chain G:



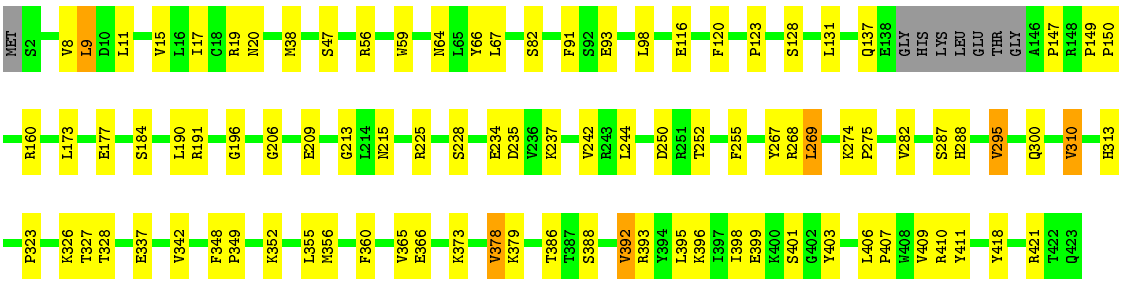
- Molecule 2: AP-1 complex subunit sigma-1A

Chain S:



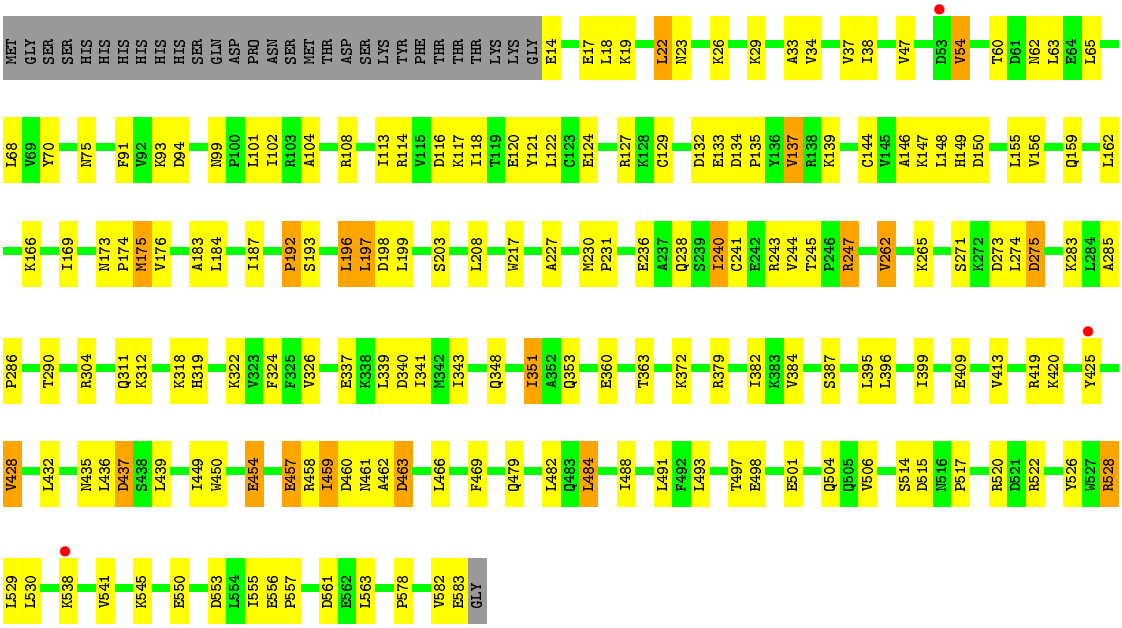
- Molecule 3: AP-1 complex subunit mu-1

Chain M:



• Molecule 4: AP-1 complex subunit beta-1

Chain B:

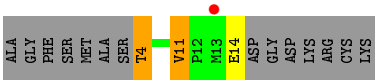


• Molecule 5: Protein Vpu

Chain V:

• Molecule 6: Bone marrow stromal antigen 2

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	160.54Å 160.54Å 118.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 48.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.00) 99.4 (48.76-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.186 , 0.229 0.189 , 0.232	Depositor DCC
R_{free} test set	3036 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	89.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.8	EDS
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 59937 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13940	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	G	0.62	1/4710 (0.0%)	0.79	5/6357 (0.1%)
2	S	0.72	0/1252	0.77	1/1674 (0.1%)
3	M	0.78	0/3450	0.74	2/4662 (0.0%)
4	B	0.68	1/4579 (0.0%)	0.73	4/6210 (0.1%)
5	V	0.84	0/77	0.75	0/103
6	T	0.76	0/95	0.90	0/128
All	All	0.69	2/14163 (0.0%)	0.76	12/19134 (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
4	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	528	ARG	NE-CZ	20.28	1.59	1.33
1	G	83	ARG	CZ-NH2	-11.33	1.18	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	83	ARG	NE-CZ-NH1	26.94	133.77	120.30
4	B	528	ARG	NE-CZ-NH2	-19.83	110.39	120.30
1	G	83	ARG	NE-CZ-NH2	-18.02	111.29	120.30
4	B	528	ARG	CD-NE-CZ	-8.26	112.03	123.60
1	G	221	ARG	NE-CZ-NH1	5.91	123.25	120.30
4	B	528	ARG	NE-CZ-NH1	5.41	123.00	120.30
3	M	67	LEU	CB-CG-CD1	-5.37	101.88	111.00
4	B	530	LEU	CB-CG-CD2	5.36	120.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	406	LEU	CB-CG-CD1	-5.27	102.05	111.00
3	M	38	MET	CG-SD-CE	5.26	108.62	100.20
1	G	147	LYS	CD-CE-NZ	5.23	123.73	111.70
2	S	21	LEU	CB-CG-CD1	-5.14	102.27	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	528	ARG	Sidechain

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	G	4645	0	4768	121	0
2	S	1231	0	1259	27	0
3	M	3370	0	3386	55	0
4	B	4509	0	4645	108	0
5	V	78	0	70	2	0
6	T	93	0	82	3	0
7	B	2	0	0	0	0
7	G	4	0	0	0	0
7	M	5	0	0	0	0
7	S	3	0	0	0	0
All	All	13940	0	14210	284	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 10.

All (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:149:PRO:HD3	4:B:101:LEU:HB2	1.50	0.94
2:S:11:ARG:HH22	5:V:59:ASP:HB2	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:11:ARG:NH2	5:V:59:ASP:HB2	1.88	0.88
3:M:410:ARG:HH22	6:T:4:THR:HA	1.40	0.85
1:G:80:THR:HG23	2:S:142:GLN:HE21	1.42	0.84
2:S:56:LYS:HD3	2:S:73:GLY:HA2	1.61	0.81
4:B:493:LEU:HD21	4:B:538:LYS:HA	1.65	0.79
1:G:135:CYS:HB3	1:G:164:VAL:HG23	1.65	0.77
3:M:160:ARG:NH1	3:M:206:GLY:O	2.20	0.75
4:B:113:ILE:HG21	4:B:118:ILE:HD12	1.68	0.74
1:G:459:LEU:HG	1:G:476:ALA:HA	1.70	0.74
3:M:399:GLU:HG3	3:M:401:SER:H	1.51	0.74
1:G:268:ASN:HD21	1:G:302:GLU:H	1.36	0.73
4:B:127:ARG:NH2	4:B:159:GLN:OE1	2.23	0.72
3:M:349:PRO:HG2	3:M:352:LYS:HG3	1.74	0.69
1:G:562:ARG:HG2	4:B:522:ARG:NH1	2.09	0.68
1:G:523:ARG:HB3	1:G:559:LEU:HD11	1.76	0.68
1:G:470:GLN:HG3	1:G:522:THR:HG21	1.76	0.68
4:B:351:ILE:HD13	4:B:387:SER:HB3	1.76	0.67
3:M:173:LEU:HD11	3:M:395:LEU:HD22	1.76	0.67
1:G:10:LEU:HD13	1:G:30:GLU:HG3	1.77	0.67
4:B:348:GLN:HA	4:B:351:ILE:HD11	1.75	0.66
1:G:162:VAL:HG13	1:G:200:GLU:HG3	1.78	0.66
1:G:555:ILE:O	4:B:419:ARG:NH1	2.20	0.65
3:M:268:ARG:NH2	4:B:290:THR:OG1	2.26	0.64
1:G:251:ARG:NH1	2:S:75:ASP:OD1	2.30	0.64
1:G:454:TYR:OH	1:G:458:ARG:NH1	2.32	0.63
1:G:80:THR:HG23	2:S:142:GLN:NE2	2.13	0.62
4:B:19:LYS:O	4:B:23:ASN:ND2	2.32	0.62
1:G:282:LYS:O	1:G:286:ASN:ND2	2.31	0.62
3:M:378:VAL:HG13	3:M:418:TYR:HD2	1.64	0.62
4:B:60:THR:HG22	4:B:62:ASN:H	1.64	0.61
4:B:459:ILE:HB	4:B:462:ALA:HB2	1.82	0.61
4:B:379:ARG:NH2	4:B:553:ASP:OD2	2.33	0.61
1:G:341:ASN:HA	1:G:344:GLN:HB2	1.81	0.61
1:G:200:GLU:O	1:G:204:ARG:HG2	2.02	0.60
3:M:19:ARG:NH1	3:M:20:ASN:O	2.34	0.60
4:B:70:TYR:OH	4:B:94:ASP:OD2	2.18	0.60
3:M:93:GLU:OE2	3:M:128:SER:OG	2.18	0.60
3:M:235:ASP:OD2	3:M:237:LYS:NZ	2.35	0.60
4:B:497:THR:OG1	4:B:498:GLU:N	2.34	0.59
4:B:99:ASN:HB3	4:B:102:ILE:HG22	1.84	0.59
1:G:260:ASP:O	1:G:264:SER:OG	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:410:ARG:NH2	6:T:4:THR:HA	2.15	0.58
1:G:456:VAL:HG12	1:G:487:LEU:HD13	1.86	0.58
1:G:416:ARG:NH1	1:G:454:TYR:OH	2.36	0.58
1:G:430:GLY:O	1:G:433:VAL:HG12	2.04	0.57
4:B:343:ILE:HD13	4:B:379:ARG:HD3	1.86	0.57
1:G:420:ASP:HA	1:G:458:ARG:NH2	2.19	0.57
4:B:166:LYS:HD2	4:B:197:LEU:HD12	1.85	0.57
4:B:196:LEU:HG	4:B:198:ASP:H	1.69	0.57
1:G:182:LEU:HD12	1:G:183:LEU:HD22	1.87	0.57
1:G:206:PRO:HA	1:G:209:LEU:HD12	1.86	0.57
4:B:22:LEU:HD21	4:B:54:VAL:HG12	1.87	0.56
4:B:449:ILE:HD11	4:B:469:PHE:CD1	2.40	0.56
2:S:34:GLU:OE1	2:S:52:TRP:NE1	2.35	0.56
1:G:210:ALA:HA	1:G:213:ARG:HD2	1.87	0.56
4:B:114:ARG:NH2	4:B:150:ASP:OD2	2.38	0.56
3:M:395:LEU:HD23	3:M:407:PRO:HB3	1.87	0.56
1:G:426:LEU:HB3	1:G:472:LEU:HD23	1.88	0.56
1:G:447:ASN:ND2	1:G:588:GLU:O	2.38	0.56
1:G:351:VAL:HG11	1:G:384:GLU:HG2	1.88	0.55
4:B:304:ARG:NH1	4:B:337:GLU:OE1	2.39	0.55
3:M:373:LYS:HE2	4:B:363:THR:HG21	1.88	0.55
1:G:271:LEU:HD13	1:G:296:ILE:HG12	1.88	0.55
1:G:207:ASP:OD2	1:G:207:ASP:N	2.40	0.55
3:M:120:PHE:CD1	4:B:147:LYS:HG2	2.43	0.54
1:G:537:PHE:HE2	1:G:539:CYS:HB2	1.72	0.54
3:M:399:GLU:HG2	3:M:403:TYR:CE2	2.42	0.54
1:G:574:ASP:N	1:G:574:ASP:OD1	2.41	0.54
1:G:131:SER:HB3	1:G:134:MET:HG3	1.90	0.54
1:G:456:VAL:HG21	1:G:483:TYR:HB2	1.90	0.54
3:M:288:HIS:CE1	3:M:366:GLU:HG3	2.43	0.54
1:G:364:ARG:NE	2:S:51:GLU:OE2	2.41	0.54
1:G:330:THR:OG1	1:G:364:ARG:NH1	2.41	0.53
4:B:469:PHE:HB3	4:B:484:LEU:HD11	1.91	0.53
4:B:26:LYS:HD2	4:B:29:LYS:HD3	1.90	0.53
1:G:420:ASP:HA	1:G:458:ARG:HH22	1.74	0.53
4:B:227:ALA:HB2	4:B:262:VAL:HG12	1.90	0.53
3:M:378:VAL:HG13	3:M:418:TYR:CD2	2.42	0.53
4:B:409:GLU:O	4:B:413:VAL:HG12	2.09	0.53
1:G:489:SER:O	1:G:491:GLN:N	2.38	0.52
1:G:12:ARG:O	1:G:16:THR:HG23	2.09	0.52
1:G:219:LEU:HD11	1:G:253:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:38:ILE:HD13	4:B:68:LEU:HG	1.92	0.52
1:G:502:GLU:HB3	1:G:537:PHE:CZ	2.45	0.52
3:M:250:ASP:OD2	3:M:252:THR:OG1	2.21	0.52
1:G:564:VAL:HG21	4:B:545:LYS:HG2	1.92	0.52
3:M:244:LEU:HD12	4:B:247:ARG:NH2	2.25	0.52
3:M:184:SER:HB3	3:M:190:LEU:HD21	1.92	0.52
4:B:450:TRP:CZ2	4:B:454:GLU:HG3	2.45	0.52
4:B:129:CYS:HA	4:B:132:ASP:HB2	1.92	0.52
2:S:71:ILE:HG12	2:S:80:THR:HG21	1.92	0.52
2:S:34:GLU:OE2	2:S:53:ARG:NH1	2.43	0.51
1:G:548:VAL:HG21	1:G:566:TYR:HB2	1.92	0.51
4:B:522:ARG:NH2	4:B:526:TYR:OH	2.44	0.51
4:B:245:THR:HG21	4:B:283:LYS:HD2	1.93	0.51
4:B:322:LYS:NZ	4:B:353:GLN:OE1	2.44	0.51
4:B:175:MET:N	4:B:175:MET:SD	2.84	0.51
1:G:542:ASN:HA	1:G:545:LYS:HE3	1.93	0.50
3:M:287:SER:HB3	3:M:288:HIS:HD2	1.75	0.50
4:B:124:GLU:OE1	4:B:127:ARG:NH1	2.44	0.50
1:G:518:SER:O	1:G:523:ARG:NH1	2.45	0.50
4:B:275:ASP:OD1	4:B:275:ASP:N	2.45	0.50
1:G:208:MET:HG3	1:G:212:PHE:HE1	1.76	0.50
1:G:155:LYS:HB2	1:G:193:THR:HG21	1.94	0.49
4:B:425:TYR:HB2	4:B:458:ARG:NE	2.27	0.49
4:B:382:ILE:HG13	4:B:420:LYS:HD2	1.95	0.49
3:M:225:ARG:O	3:M:228:SER:OG	2.29	0.49
3:M:91:PHE:HB3	3:M:98:LEU:HD13	1.94	0.49
1:G:562:ARG:HH21	4:B:482:LEU:CD2	2.26	0.49
1:G:409:GLU:HG2	1:G:444:LEU:HD11	1.94	0.49
1:G:470:GLN:OE1	1:G:518:SER:HA	2.12	0.49
3:M:177:GLU:OE1	3:M:388:SER:HB3	2.11	0.49
4:B:14:GLU:HG2	4:B:17:GLU:H	1.78	0.49
2:S:32:VAL:O	2:S:36:MET:HB2	2.12	0.48
3:M:9:LEU:HD12	3:M:15:VAL:HA	1.94	0.48
4:B:196:LEU:HD21	4:B:198:ASP:HB3	1.95	0.48
1:G:386:LEU:HD11	1:G:424:ARG:HG2	1.96	0.48
4:B:149:HIS:HA	4:B:156:VAL:HG21	1.95	0.48
1:G:556:ASP:HB3	1:G:559:LEU:HB2	1.95	0.48
2:S:76:ASN:O	2:S:80:THR:HG23	2.14	0.48
3:M:8:VAL:HB	3:M:17:ILE:HG22	1.94	0.48
1:G:340:HIS:CE1	1:G:344:GLN:HE21	2.32	0.48
1:G:293:VAL:HG11	1:G:313:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:LEU:HD23	1:G:256:LEU:HD23	1.96	0.48
1:G:191:LEU:O	1:G:195:VAL:HG23	2.13	0.48
1:G:485:ASP:OD2	1:G:486:LEU:N	2.47	0.48
1:G:73:LEU:HB3	1:G:81:ASP:O	2.13	0.48
1:G:344:GLN:NE2	1:G:374:ASN:HD21	2.12	0.48
3:M:327:THR:HG22	3:M:356:MET:HG3	1.94	0.48
1:G:115:THR:HG21	2:S:141:LEU:HD21	1.96	0.47
2:S:93:LYS:HG2	2:S:132:LEU:HD13	1.95	0.47
4:B:183:ALA:O	4:B:187:ILE:HG12	2.14	0.47
1:G:453:ALA:O	1:G:457:GLN:HG2	2.14	0.47
3:M:196:GLY:HA3	3:M:267:TYR:CZ	2.49	0.47
3:M:323:PRO:HB3	3:M:360:PHE:CE2	2.49	0.47
1:G:302:GLU:HG2	1:G:304:GLY:H	1.80	0.47
4:B:578:PRO:O	4:B:582:VAL:HG13	2.14	0.47
4:B:501:GLU:CD	4:B:501:GLU:H	2.18	0.47
1:G:323:ASN:HB3	2:S:49:PHE:HE1	1.79	0.47
4:B:162:LEU:HD12	4:B:162:LEU:H	1.80	0.47
4:B:227:ALA:O	4:B:265:LYS:NZ	2.37	0.47
3:M:9:LEU:HB2	3:M:66:TYR:HB2	1.97	0.47
4:B:241:CYS:O	4:B:245:THR:OG1	2.27	0.47
4:B:139:LYS:HB3	4:B:176:VAL:HA	1.97	0.47
4:B:122:LEU:HD23	4:B:148:LEU:HD11	1.96	0.47
3:M:242:VAL:HA	3:M:255:PHE:HB3	1.96	0.47
3:M:191[B]:ARG:HD3	4:B:322:LYS:O	2.15	0.47
3:M:421:ARG:NH1	4:B:360:GLU:HG2	2.30	0.47
4:B:318:LYS:HD2	4:B:319:HIS:CE1	2.50	0.46
1:G:111:LEU:O	1:G:119:GLN:NE2	2.33	0.46
4:B:515:ASP:OD2	4:B:515:ASP:N	2.49	0.46
1:G:152:TYR:HA	1:G:155:LYS:HE2	1.98	0.46
1:G:11:ILE:O	1:G:15:ARG:HG3	2.16	0.46
4:B:514:SER:O	4:B:520:ARG:NH1	2.48	0.46
4:B:33:ALA:O	4:B:37:VAL:HG23	2.15	0.46
1:G:558:GLU:OE2	4:B:482:LEU:HB3	2.16	0.46
4:B:18:LEU:O	4:B:22:LEU:HB2	2.16	0.46
2:S:49:PHE:CE2	2:S:77:GLU:HB3	2.50	0.46
4:B:459:ILE:HG22	4:B:461:ASN:OD1	2.15	0.46
4:B:37:VAL:HG13	4:B:47:VAL:HG21	1.97	0.45
3:M:386:THR:HG23	3:M:411:TYR:HB3	1.98	0.45
2:S:119:MET:O	2:S:121:GLY:N	2.49	0.45
3:M:295:VAL:HG13	3:M:356:MET:HB3	1.98	0.45
1:G:94:ASP:N	1:G:94:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:3:ARG:HH11	2:S:55:LEU:HD11	1.82	0.45
1:G:104:THR:HG23	1:G:138:LEU:HD21	1.99	0.45
4:B:271:SER:HB3	4:B:274:LEU:HD23	1.99	0.45
1:G:248:ARG:HA	1:G:248:ARG:HD3	1.75	0.45
1:G:68:LEU:HA	1:G:71:LEU:HD23	1.97	0.45
1:G:439:PRO:HB3	4:B:517:PRO:HD3	1.99	0.45
1:G:289:LEU:HD21	1:G:312:ILE:HD12	1.99	0.45
3:M:234:GLU:HG2	3:M:269:LEU:HA	1.99	0.45
1:G:237:VAL:HG21	1:G:243:PRO:HG3	1.99	0.45
1:G:162:VAL:HG22	1:G:197:LEU:HA	1.99	0.45
3:M:275:PRO:O	3:M:300:GLN:NE2	2.46	0.45
4:B:488:ILE:HD12	4:B:506:VAL:HG21	1.99	0.45
3:M:147:PRO:HD2	4:B:63:LEU:HD23	1.98	0.45
3:M:392:VAL:HG11	3:M:409:VAL:HG21	1.99	0.44
4:B:236:GLU:O	4:B:240:ILE:HG23	2.17	0.44
3:M:407:PRO:HG2	6:T:11:VAL:HG13	1.98	0.44
1:G:331:SER:O	1:G:335:THR:HG22	2.18	0.44
4:B:60:THR:HG21	4:B:65:LEU:HD23	1.98	0.44
3:M:244:LEU:HD12	4:B:247:ARG:HH21	1.81	0.44
1:G:408:ALA:O	1:G:412:ALA:HB2	2.18	0.44
2:S:7:LEU:HG	2:S:16:LEU:HB3	1.98	0.44
3:M:11:LEU:HD21	3:M:64:ASN:HA	1.99	0.44
4:B:466:LEU:HD12	4:B:491:LEU:HD22	2.00	0.44
1:G:463:ILE:HG22	1:G:472:LEU:HD13	2.00	0.43
2:S:77:GLU:OE1	2:S:77:GLU:N	2.51	0.43
1:G:327:VAL:HG21	2:S:78:LEU:HD11	1.99	0.43
3:M:123:PRO:HB2	4:B:217:TRP:CG	2.53	0.43
1:G:160:CYS:O	1:G:164:VAL:HG12	2.18	0.43
1:G:487:LEU:O	1:G:500:VAL:HG21	2.19	0.43
3:M:215:ASN:N	3:M:215:ASN:OD1	2.45	0.43
4:B:230:MET:SD	4:B:231:PRO:HD2	2.57	0.43
1:G:273:GLN:O	1:G:277:ASN:HB2	2.19	0.43
4:B:395:LEU:O	4:B:399:ILE:HG13	2.19	0.43
1:G:577:ARG:HG2	1:G:577:ARG:H	1.53	0.43
1:G:2:PRO:HA	1:G:3:ALA:HA	1.72	0.43
3:M:396:LYS:HD3	3:M:398:ILE:HD11	2.01	0.43
3:M:137:GLN:OE1	3:M:137:GLN:N	2.46	0.43
1:G:513:LEU:HD23	1:G:513:LEU:HA	1.88	0.43
1:G:526:ALA:O	1:G:530:ILE:HG13	2.18	0.43
4:B:311:GLN:HE22	4:B:555:ILE:HG13	1.82	0.43
4:B:556:GLU:HA	4:B:557:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:541:VAL:O	1:G:544:ILE:HG12	2.19	0.43
4:B:93:LYS:HD3	4:B:93:LYS:HA	1.91	0.43
1:G:23:GLU:O	1:G:27:ILE:HG12	2.19	0.43
4:B:435:ASN:C	4:B:437:ASP:H	2.23	0.42
4:B:324:PHE:CE2	4:B:341:ILE:HG21	2.54	0.42
3:M:310:VAL:HA	3:M:379:LYS:O	2.19	0.42
1:G:128:CYS:HG	2:S:20:TYR:HE2	1.67	0.42
4:B:396:LEU:HD11	4:B:428:VAL:HG23	2.01	0.42
4:B:146:ALA:HA	4:B:187:ILE:HD11	2.01	0.42
4:B:116:ASP:O	4:B:120:GLU:HG3	2.19	0.42
3:M:213:GLY:O	3:M:393:ARG:N	2.43	0.42
3:M:116:GLU:OE1	4:B:108:ARG:NH2	2.51	0.42
1:G:232:SER:O	1:G:234:GLU:N	2.44	0.42
4:B:144:CYS:O	4:B:147:LYS:HB2	2.19	0.42
1:G:531:MET:O	1:G:581:LEU:HD13	2.19	0.42
1:G:265:GLU:O	1:G:268:ASN:HB2	2.20	0.42
1:G:438:VAL:N	1:G:439:PRO:HD2	2.35	0.42
3:M:209:GLU:HB3	3:M:398:ILE:HB	2.02	0.42
4:B:339:LEU:HA	4:B:339:LEU:HD23	1.85	0.42
1:G:413:PRO:HD2	1:G:417:TRP:CE3	2.55	0.42
4:B:134:ASP:HA	4:B:135:PRO:HD3	1.85	0.42
4:B:244:VAL:O	4:B:247:ARG:HB2	2.20	0.41
2:S:50:LEU:HG	2:S:57:VAL:HB	2.01	0.41
1:G:206:PRO:O	1:G:209:LEU:HB2	2.20	0.41
4:B:437:ASP:OD2	4:B:437:ASP:N	2.53	0.41
2:S:108:GLU:HG3	2:S:108:GLU:H	1.38	0.41
4:B:208:LEU:HG	4:B:243:ARG:HE	1.84	0.41
4:B:449:ILE:HD11	4:B:469:PHE:HD1	1.84	0.41
1:G:536:ARG:NH1	1:G:581:LEU:O	2.44	0.41
1:G:38:PHE:CE2	1:G:69:GLU:HG2	2.55	0.41
3:M:313:HIS:ND1	3:M:342:VAL:HG22	2.35	0.41
1:G:442:ILE:HD12	4:B:517:PRO:HG2	2.01	0.41
1:G:389:LEU:O	1:G:392:CYS:HB2	2.20	0.41
1:G:508:ILE:HA	1:G:508:ILE:HD12	1.94	0.41
4:B:133:GLU:H	4:B:133:GLU:HG2	1.57	0.41
1:G:377:ASN:OD1	1:G:377:ASN:N	2.46	0.41
1:G:287:ALA:HB2	2:S:78:LEU:HB2	2.03	0.41
1:G:223:LEU:O	1:G:227:ILE:HG13	2.20	0.41
4:B:156:VAL:HG23	4:B:156:VAL:H	1.60	0.41
1:G:15:ARG:HD3	1:G:15:ARG:HH11	1.73	0.41
2:S:43:LYS:HA	2:S:44:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:173:ASN:HA	4:B:174:PRO:HD2	1.87	0.41
1:G:74:ILE:O	1:G:82:LYS:NZ	2.53	0.41
1:G:172:MET:HE3	1:G:172:MET:HB2	1.98	0.41
3:M:149:PRO:HA	3:M:150:PRO:HD3	1.93	0.41
1:G:470:GLN:HG2	1:G:519:THR:HG23	2.01	0.41
2:S:3:ARG:NH1	2:S:55:LEU:HD21	2.35	0.41
4:B:463:ASP:HA	4:B:491:LEU:HD21	2.03	0.41
3:M:47:SER:O	3:M:59:TRP:NE1	2.52	0.41
4:B:285:ALA:HB3	4:B:286:PRO:HD3	2.03	0.41
1:G:167:LYS:HD3	1:G:167:LYS:HA	1.91	0.41
4:B:199:LEU:HB2	4:B:203:SER:OG	2.21	0.41
3:M:328:THR:HG23	3:M:355:LEU:HB2	2.02	0.41
4:B:312:LYS:NZ	4:B:561:ASP:OD1	2.48	0.41
4:B:117:LYS:O	4:B:121:TYR:HD2	2.04	0.41
1:G:519:THR:OG1	1:G:522:THR:HG23	2.21	0.41
4:B:38:ILE:CD1	4:B:68:LEU:HG	2.50	0.41
1:G:31:CYS:HB3	1:G:35:ARG:NH2	2.36	0.41
1:G:492:CYS:N	1:G:497:PRO:HG3	2.36	0.41
1:G:322:LYS:O	1:G:361:ILE:HD11	2.20	0.41
1:G:268:ASN:ND2	1:G:302:GLU:H	2.12	0.40
4:B:459:ILE:H	4:B:459:ILE:HG12	1.65	0.40
4:B:208:LEU:HD12	4:B:243:ARG:HB3	2.03	0.40
4:B:104:ALA:HB2	4:B:137:VAL:HA	2.03	0.40
1:G:123:LEU:HD13	1:G:156:LYS:HB2	2.03	0.40
1:G:137:ASP:N	1:G:137:ASP:OD2	2.54	0.40
1:G:316:PHE:HB3	1:G:328:ALA:HB2	2.03	0.40
1:G:220:VAL:HG13	1:G:270:ILE:HG21	2.02	0.40
4:B:169:ILE:HD11	4:B:184:LEU:HD22	2.03	0.40
1:G:225:ASN:O	1:G:229:SER:N	2.55	0.40
1:G:268:ASN:OD1	1:G:301:SER:HB2	2.21	0.40
1:G:215:LEU:HD12	1:G:219:LEU:HD23	2.03	0.40
1:G:94:ASP:OD2	1:G:96:ARG:HB2	2.21	0.40
4:B:192:PRO:HB2	4:B:193:SER:H	1.76	0.40
4:B:457:GLU:H	4:B:457:GLU:CD	2.25	0.40
4:B:457:GLU:OE2	4:B:457:GLU:N	2.50	0.40
1:G:173:GLU:O	1:G:176:LEU:HB2	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	G	585/627 (93%)	547 (94%)	36 (6%)	2 (0%)	46 84
2	S	145/158 (92%)	142 (98%)	2 (1%)	1 (1%)	26 70
3	M	412/423 (97%)	400 (97%)	12 (3%)	0	100 100
4	B	568/600 (95%)	542 (95%)	25 (4%)	1 (0%)	52 88
5	V	8/63 (13%)	7 (88%)	1 (12%)	0	100 100
6	T	9/25 (36%)	9 (100%)	0	0	100 100
All	All	1727/1896 (91%)	1647 (95%)	76 (4%)	4 (0%)	52 88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	452	HIS
2	S	120	GLY
1	G	490	GLY
4	B	192	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	521/557 (94%)	486 (93%)	35 (7%)	20 57
2	S	135/144 (94%)	127 (94%)	8 (6%)	24 63
3	M	378/383 (99%)	362 (96%)	16 (4%)	36 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	B	509/536 (95%)	470 (92%)	39 (8%)	16 50
5	V	9/53 (17%)	7 (78%)	2 (22%)	1 5
6	T	11/21 (52%)	8 (73%)	3 (27%)	0 2
All	All	1563/1694 (92%)	1460 (93%)	103 (7%)	21 57

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

Mol	Chain	Res	Type
1	G	71	LEU
1	G	137	ASP
1	G	176	LEU
1	G	182	LEU
1	G	191	LEU
1	G	203	GLU
1	G	207	ASP
1	G	211	HIS
1	G	218	GLN
1	G	242	ASP
1	G	273	GLN
1	G	317	LEU
1	G	333	LEU
1	G	336	VAL
1	G	338	THR
1	G	341	ASN
1	G	347	ARG
1	G	349	THR
1	G	363	ARG
1	G	364	ARG
1	G	372	LEU
1	G	381	MET
1	G	386	LEU
1	G	392	CYS
1	G	445	ILE
1	G	450	GLU
1	G	451	MET
1	G	459	LEU
1	G	469	GLN
1	G	470	GLN
1	G	520	SER
1	G	541	VAL
1	G	574	ASP

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Mol	Chain	Res	Type
1	G	577	ARG
1	G	580	LEU
2	S	3	ARG
2	S	43	LYS
2	S	53	ARG
2	S	83	LEU
2	S	86	ARG
2	S	88	VAL
2	S	108	GLU
2	S	119	MET
3	M	9	LEU
3	M	56	ARG
3	M	82	SER
3	M	131	LEU
3	M	269	LEU
3	M	274	LYS
3	M	282	VAL
3	M	295	VAL
3	M	310	VAL
3	M	326	LYS
3	M	337	GLU
3	M	348	PHE
3	M	365	VAL
3	M	378	VAL
3	M	392	VAL
3	M	406	LEU
4	B	22	LEU
4	B	34	VAL
4	B	54	VAL
4	B	75	ASN
4	B	91	PHE
4	B	137	VAL
4	B	155	LEU
4	B	175	MET
4	B	196	LEU
4	B	197	LEU
4	B	238	GLN
4	B	240	ILE
4	B	247	ARG
4	B	262	VAL
4	B	273	ASP
4	B	275	ASP

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Mol	Chain	Res	Type
4	B	326	VAL
4	B	340	ASP
4	B	351	ILE
4	B	372	LYS
4	B	384	VAL
4	B	428	VAL
4	B	432	LEU
4	B	436	LEU
4	B	437	ASP
4	B	439	LEU
4	B	454	GLU
4	B	457	GLU
4	B	459	ILE
4	B	460	ASP
4	B	463	ASP
4	B	479	GLN
4	B	484	LEU
4	B	504	GLN
4	B	529	LEU
4	B	541	VAL
4	B	550	GLU
4	B	563	LEU
4	B	583	GLU
5	V	61	GLU
5	V	68	GLU
6	T	4	THR
6	T	11	VAL
6	T	14	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	340	HIS
1	G	374	ASN
4	B	195	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	G	587/627 (93%)	-0.27	3 (0%) 91 76	55, 126, 180, 212	0
2	S	147/158 (93%)	-0.43	0 100 100	55, 90, 119, 170	0
3	M	415/423 (98%)	-0.43	0 100 100	47, 75, 113, 163	0
4	B	570/600 (95%)	-0.31	3 (0%) 91 76	58, 107, 168, 224	0
5	V	10/63 (15%)	-0.27	0 100 100	83, 87, 135, 144	0
6	T	11/25 (44%)	0.51	1 (9%) 11 4	86, 111, 135, 142	0
All	All	1740/1896 (91%)	-0.33	7 (0%) 93 80	47, 103, 169, 224	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	278	THR	3.3
4	B	53	ASP	2.3
4	B	538	LYS	2.3
4	B	425	TYR	2.1
1	G	135	CYS	2.1
6	T	13	MET	2.0
1	G	461	LYS	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.