Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 02:05 PM JST

PDB ID	:	6JCB
Title	:	Crystal structure of aminotransferase CrmG from Actinoalloteichus sp. WH1-2216-6 in C2 space group
Authors	:	Xu, J.; Liu, J.
Deposited on	:	2019-01-28
Resolution	:	2.85 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 ⓘ 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 ⓘ) were used in the production of this report:

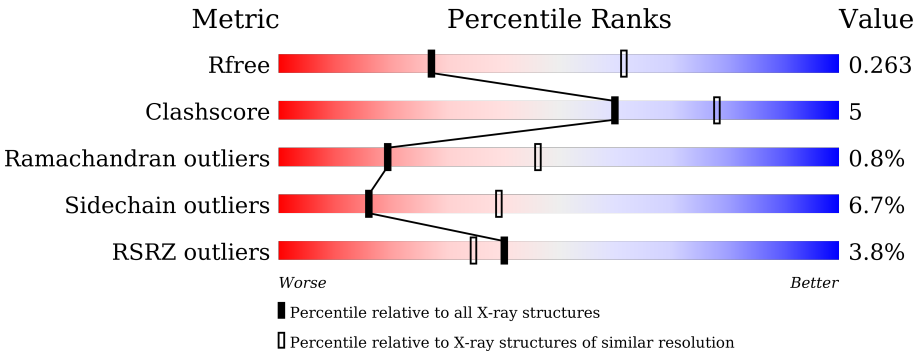
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	523	2% 79% 12% • 7%
1	B	523	5% 79% 11% • 8%
1	C	523	5% 81% 11% • 7%
1	D	523	2% 80% 11% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15140 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 CrmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3752	2341	680	720	11			
1	C	487	Total	C	N	O	S	0	0	0
			3759	2348	681	719	11			
1	B	483	Total	C	N	O	S	0	0	0
			3735	2331	677	716	11			
1	D	489	Total	C	N	O	S	0	0	0
			3775	2357	685	722	11			

- Molecule 2 is water.

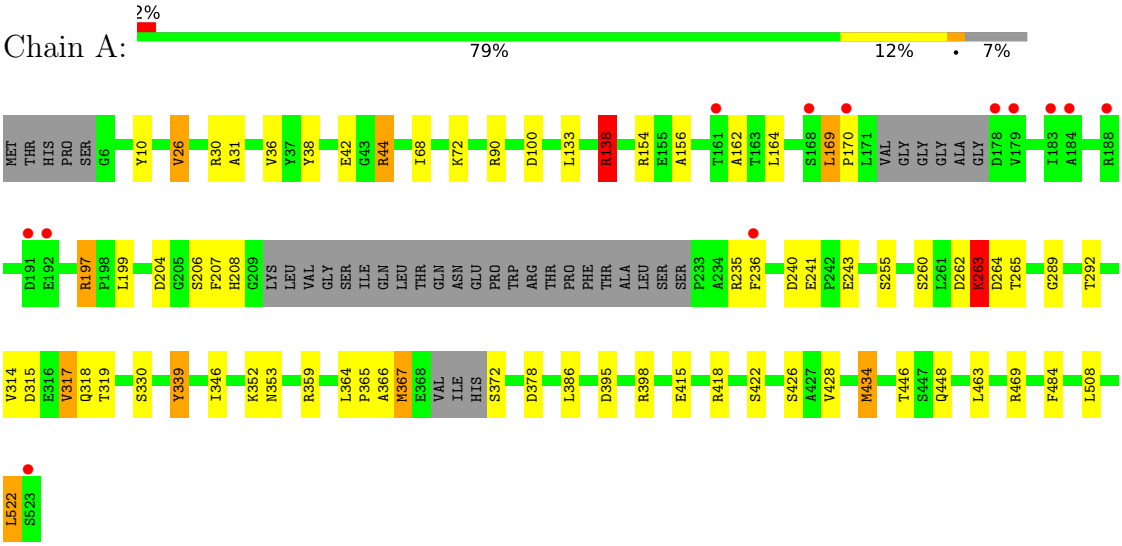
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	C	21	Total	O	0	0
			21	21		
2	B	23	Total	O	0	0
			23	23		
2	D	31	Total	O	0	0
			31	31		

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.

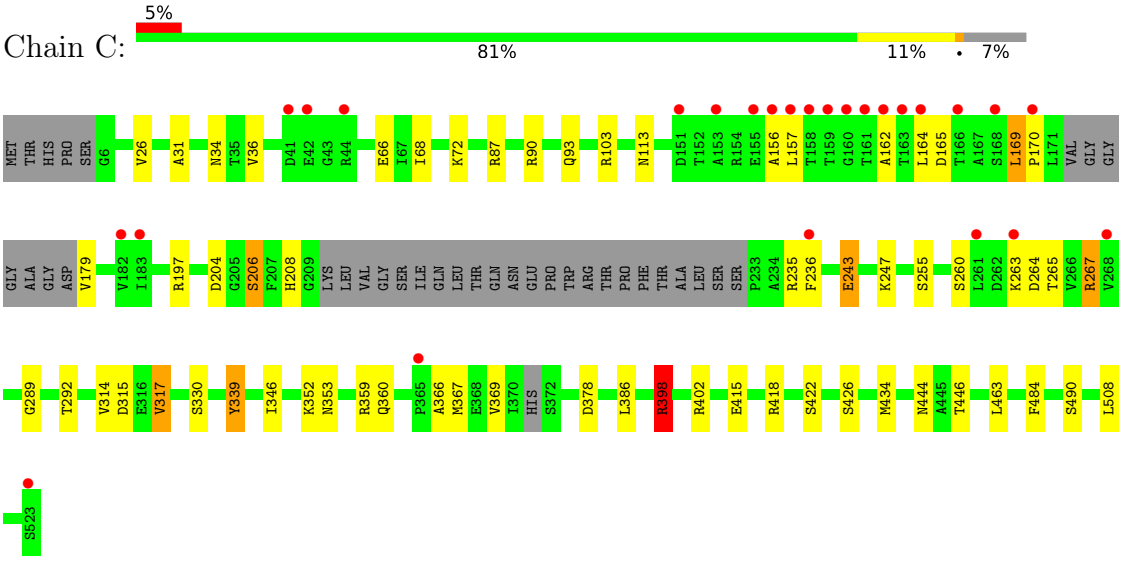
• Molecule 1: CrmG

Chain A:



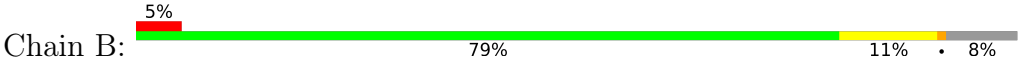
• Molecule 1: CrmG

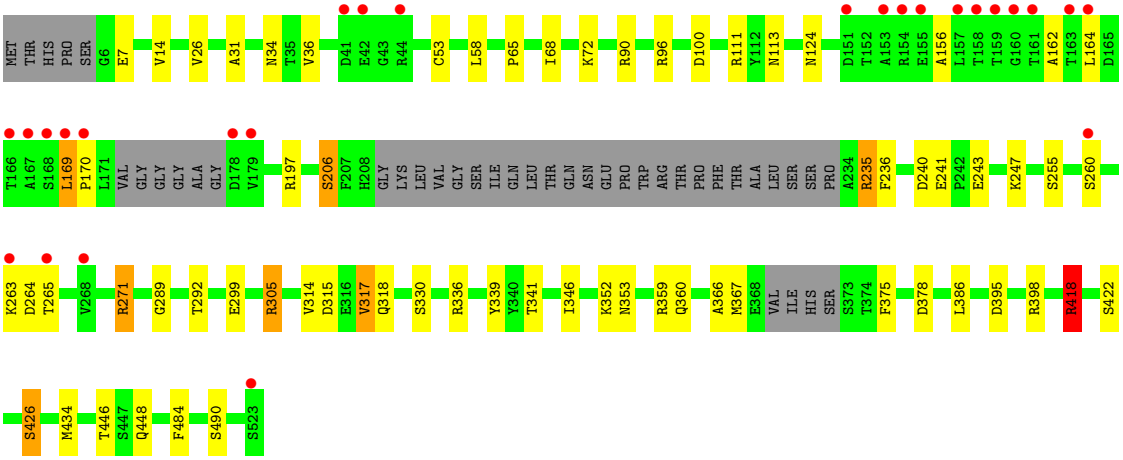
Chain C:



• Molecule 1: CrmG

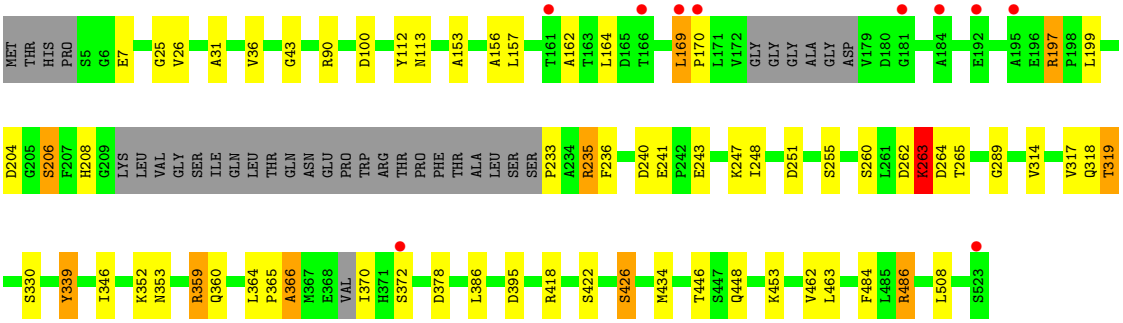
Chain B:





- Molecule 1: CrmG

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.13Å 114.83Å 156.17Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	18.00 – 2.85 38.87 – 2.85	Depositor EDS
% Data completeness (in resolution range)	92.8 (18.00-2.85) 93.2 (38.87-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.210 , 0.262 0.214 , 0.263	Depositor DCC
R_{free} test set	2342 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.105 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15140	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6448e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	0/3811	0.86	2/5153 (0.0%)
1	B	0.72	0/3793	0.87	3/5129 (0.1%)
1	C	0.72	0/3818	0.87	2/5163 (0.0%)
1	D	0.72	0/3835	0.87	2/5186 (0.0%)
All	All	0.72	0/15257	0.87	9/20631 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	305	ARG	CG-CD-NE	-5.89	99.42	111.80
1	A	138	ARG	CG-CD-NE	5.71	123.80	111.80
1	C	398	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	339	TYR	CB-CG-CD1	5.25	124.15	121.00
1	B	96	ARG	CG-CD-NE	5.24	122.80	111.80
1	B	418	ARG	CG-CD-NE	-5.20	100.88	111.80
1	D	486	ARG	CG-CD-NE	5.05	122.40	111.80
1	D	339	TYR	CB-CG-CD1	5.04	124.02	121.00
1	C	339	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3752	0	3721	41	0
1	B	3735	0	3705	34	0
1	C	3759	0	3737	32	0
1	D	3775	0	3749	42	0
2	A	44	0	0	1	0
2	B	23	0	0	0	0
2	C	21	0	0	1	0
2	D	31	0	0	1	0
All	All	15140	0	14912	138	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 5.

All (138) 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:319:THR:HA	1:A:434:MET:CE	1.89	1.01
1:A:42:GLU:HB2	1:A:44:ARG:HD3	1.45	0.98
1:B:271:ARG:HH11	1:B:271:ARG:HG2	1.27	0.98
1:D:113:ASN:ND2	1:D:360:GLN:HE21	1.78	0.80
1:C:113:ASN:ND2	1:C:360:GLN:HE21	1.79	0.79
1:B:113:ASN:ND2	1:B:360:GLN:HE21	1.80	0.78
1:A:319:THR:HA	1:A:434:MET:HE1	1.71	0.72
1:C:165:ASP:OD2	1:C:267:ARG:NH2	2.24	0.71
1:D:153:ALA:O	1:D:157:LEU:HD23	1.91	0.71
1:D:153:ALA:O	1:D:157:LEU:CD2	2.40	0.70
1:C:157:LEU:HD23	1:C:179:VAL:HG22	1.78	0.66
1:A:319:THR:HA	1:A:434:MET:HE3	1.74	0.66
1:A:314:VAL:HG11	1:A:330:SER:HB3	1.77	0.65
1:A:30:ARG:NH2	1:D:43:GLY:O	2.28	0.65
1:B:314:VAL:HG11	1:B:330:SER:HB3	1.80	0.62
1:C:314:VAL:HG11	1:C:330:SER:HB3	1.80	0.62
1:B:271:ARG:HG2	1:B:271:ARG:NH1	2.02	0.61
1:A:138:ARG:HH21	1:A:138:ARG:HG2	1.66	0.61
1:D:314:VAL:HG11	1:D:330:SER:HB3	1.83	0.59
1:A:415:GLU:OE2	1:A:418:ARG:NH1	2.36	0.59
1:B:305:ARG:NH2	1:B:336:ARG:O	2.36	0.58
1:C:113:ASN:ND2	1:C:360:GLN:NE2	2.51	0.58
1:B:113:ASN:ND2	1:B:360:GLN:NE2	2.51	0.58
1:D:453:LYS:HD3	1:D:462:VAL:HG21	1.86	0.58
1:A:138:ARG:HH21	1:A:138:ARG:CG	2.18	0.57
1:C:415:GLU:OE2	1:C:418:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:THR:HB	1:D:434:MET:HE1	1.87	0.57
1:A:204:ASP:O	2:A:601:HOH:O	2.17	0.57
1:D:247:LYS:HE3	1:D:251:ASP:OD2	2.05	0.56
1:D:370:ILE:O	1:D:370:ILE:HG13	2.05	0.56
1:C:169:LEU:N	1:C:170:PRO:CD	2.69	0.56
1:C:157:LEU:HD21	1:C:164:LEU:HB2	1.88	0.56
1:C:463:LEU:HG	1:C:508:LEU:HD11	1.88	0.56
1:A:10:TYR:CE1	1:B:111:ARG:HD3	2.41	0.56
1:D:169:LEU:N	1:D:170:PRO:CD	2.69	0.55
1:A:169:LEU:N	1:A:170:PRO:CD	2.69	0.55
1:B:271:ARG:HH11	1:B:271:ARG:CG	2.09	0.55
1:D:113:ASN:ND2	1:D:360:GLN:NE2	2.53	0.55
1:C:378:ASP:OD2	1:D:352:LYS:CE	2.55	0.55
1:B:169:LEU:N	1:B:170:PRO:CD	2.69	0.55
1:B:418:ARG:NH1	1:B:426:SER:O	2.41	0.54
1:D:164:LEU:HD11	1:D:169:LEU:HD21	1.91	0.53
1:C:164:LEU:HD11	1:C:169:LEU:HD21	1.90	0.53
1:C:157:LEU:HD23	1:C:179:VAL:CG2	2.40	0.52
1:D:204:ASP:O	2:D:601:HOH:O	2.19	0.52
1:B:164:LEU:HD11	1:B:169:LEU:HD21	1.90	0.52
1:D:162:ALA:HA	1:D:264:ASP:O	2.10	0.52
1:B:124:ASN:ND2	1:B:341:THR:HG21	2.25	0.52
1:A:162:ALA:HA	1:A:264:ASP:O	2.10	0.51
1:B:162:ALA:HA	1:B:264:ASP:O	2.10	0.51
1:C:162:ALA:HA	1:C:264:ASP:O	2.10	0.51
1:B:90:ARG:HD3	1:B:386:LEU:HD12	1.92	0.51
1:A:262:ASP:O	1:A:263:LYS:HG2	2.10	0.51
1:A:164:LEU:HD11	1:A:169:LEU:HD21	1.92	0.51
1:D:366:ALA:O	1:D:370:ILE:N	2.43	0.51
1:D:153:ALA:O	1:D:157:LEU:HD22	2.10	0.50
1:B:124:ASN:HD22	1:B:341:THR:HG21	1.75	0.50
1:D:113:ASN:HD21	1:D:360:GLN:HE21	1.59	0.50
1:A:90:ARG:HD3	1:A:386:LEU:HD12	1.94	0.50
1:C:90:ARG:HD3	1:C:386:LEU:HD12	1.94	0.50
1:A:352:LYS:HE3	1:B:378:ASP:OD2	2.12	0.49
1:C:113:ASN:HD21	1:C:360:GLN:NE2	2.10	0.49
1:C:204:ASP:O	2:C:601:HOH:O	2.20	0.48
1:B:235:ARG:HH11	1:B:235:ARG:HA	1.79	0.48
1:C:352:LYS:CE	1:D:378:ASP:OD2	2.62	0.48
1:D:113:ASN:HD21	1:D:360:GLN:NE2	2.10	0.48
1:B:346:ILE:HG22	1:B:353:ASN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HD3	1:D:386:LEU:HD12	1.97	0.47
1:A:206:SER:O	1:A:236:PHE:CE2	2.68	0.47
1:B:68:ILE:O	1:B:72:LYS:HG3	2.15	0.47
1:C:68:ILE:O	1:C:72:LYS:HG3	2.15	0.47
1:D:262:ASP:O	1:D:263:LYS:HG2	2.15	0.47
1:D:418:ARG:NH1	1:D:426:SER:O	2.47	0.46
1:C:66:GLU:HG2	1:B:65:PRO:HB3	1.97	0.46
1:B:113:ASN:HD21	1:B:360:GLN:NE2	2.12	0.46
1:B:31:ALA:HB2	1:B:36:VAL:HG12	1.98	0.45
1:C:164:LEU:HD13	1:C:164:LEU:O	2.17	0.45
1:C:315:ASP:OD1	1:C:317:VAL:HB	2.16	0.45
1:D:235:ARG:HH21	1:D:248:ILE:HG21	1.82	0.45
1:A:317:VAL:HG12	1:A:318:GLN:HG2	1.98	0.45
1:A:315:ASP:OD1	1:A:317:VAL:HB	2.16	0.45
1:A:346:ILE:HG22	1:A:353:ASN:HB3	1.97	0.45
1:B:206:SER:O	1:B:236:PHE:CE2	2.70	0.45
1:A:206:SER:O	1:A:236:PHE:HE2	2.00	0.45
1:D:206:SER:O	1:D:236:PHE:CE2	2.70	0.45
1:C:31:ALA:HB2	1:C:36:VAL:HG12	1.98	0.44
1:B:315:ASP:OD1	1:B:317:VAL:HB	2.17	0.44
1:C:378:ASP:OD2	1:D:352:LYS:HE3	2.18	0.44
1:B:164:LEU:O	1:B:164:LEU:HD13	2.17	0.44
1:D:346:ILE:HG22	1:D:353:ASN:HB3	1.98	0.44
1:D:31:ALA:HB2	1:D:36:VAL:HG12	1.98	0.44
1:A:289:GLY:HA3	1:A:484:PHE:CD2	2.53	0.44
1:A:378:ASP:OD2	1:B:352:LYS:CE	2.66	0.43
1:C:346:ILE:HG22	1:C:353:ASN:HB3	2.00	0.43
1:D:206:SER:O	1:D:236:PHE:HE2	2.01	0.43
1:A:42:GLU:HB2	1:A:44:ARG:CD	2.31	0.43
1:A:469:ARG:NH1	1:A:522:LEU:HD21	2.33	0.43
1:C:206:SER:O	1:C:236:PHE:CE2	2.72	0.43
1:B:317:VAL:HG12	1:B:318:GLN:HG2	2.00	0.43
1:A:207:PHE:CD2	1:A:236:PHE:HZ	2.37	0.43
1:A:31:ALA:HB2	1:A:36:VAL:HG12	1.99	0.43
1:A:68:ILE:O	1:A:72:LYS:HG3	2.18	0.43
1:A:463:LEU:HB3	1:A:508:LEU:HD21	2.01	0.43
1:D:112:TYR:CE1	1:D:359:ARG:HG3	2.53	0.43
1:D:289:GLY:HA3	1:D:484:PHE:CD2	2.54	0.43
1:D:164:LEU:HD13	1:D:164:LEU:O	2.19	0.42
1:C:289:GLY:HA3	1:C:484:PHE:CD2	2.54	0.42
1:C:87:ARG:HD2	1:D:25:GLY:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:THR:HB	1:D:434:MET:CE	2.49	0.42
1:B:289:GLY:HA3	1:B:484:PHE:CD2	2.54	0.42
1:C:264:ASP:OD1	1:C:265:THR:HG22	2.19	0.42
1:D:199:LEU:HD12	1:D:199:LEU:HA	1.93	0.42
1:D:264:ASP:OD1	1:D:265:THR:HG22	2.19	0.42
1:B:206:SER:O	1:B:236:PHE:HE2	2.02	0.42
1:A:42:GLU:HG3	1:A:44:ARG:HH11	1.84	0.42
1:A:197:ARG:O	1:A:197:ARG:HD3	2.20	0.42
1:D:235:ARG:NH1	1:D:236:PHE:O	2.53	0.42
1:C:398:ARG:CB	1:C:398:ARG:HH21	2.33	0.41
1:B:264:ASP:OD1	1:B:265:THR:HG22	2.20	0.41
1:A:42:GLU:HG3	1:A:44:ARG:NH1	2.35	0.41
1:A:264:ASP:OD1	1:A:265:THR:HG22	2.19	0.41
1:A:352:LYS:HE2	1:B:375:PHE:O	2.21	0.41
1:D:463:LEU:HB3	1:D:508:LEU:HD21	2.03	0.41
1:A:164:LEU:HD13	1:A:164:LEU:O	2.20	0.41
1:D:197:ARG:HG3	1:D:233:PRO:HB3	2.03	0.41
1:A:169:LEU:N	1:A:170:PRO:HD2	2.35	0.41
1:C:34:ASN:ND2	1:C:490:SER:OG	2.53	0.41
1:D:317:VAL:HG23	1:D:318:GLN:HG2	2.01	0.41
1:D:486:ARG:HH21	1:D:486:ARG:HG3	1.85	0.41
1:B:53:CYS:HB3	1:B:58:LEU:HB2	2.03	0.40
1:A:197:ARG:NH2	1:A:199:LEU:HD13	2.35	0.40
1:A:364:LEU:HA	1:A:365:PRO:HD3	1.95	0.40
1:A:365:PRO:HB3	1:B:14:VAL:HG21	2.02	0.40
1:A:26:VAL:CG2	1:A:38:TYR:CG	3.05	0.40
1:C:243:GLU:H	1:C:243:GLU:HG3	1.67	0.40
1:C:444:ASN:HD22	1:C:444:ASN:HA	1.62	0.40
1:B:34:ASN:ND2	1:B:490:SER:OG	2.54	0.40
1:D:364:LEU:HA	1:D:365:PRO:HD3	1.97	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	478/523 (91%)	446 (93%)	28 (6%)	4 (1%)	19	46
1	B	475/523 (91%)	444 (94%)	27 (6%)	4 (1%)	19	46
1	C	479/523 (92%)	448 (94%)	28 (6%)	3 (1%)	25	53
1	D	481/523 (92%)	449 (93%)	28 (6%)	4 (1%)	19	46
All	All	1913/2092 (91%)	1787 (93%)	111 (6%)	15 (1%)	19	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ALA
1	A	366	ALA
1	A	367	MET
1	C	156	ALA
1	C	366	ALA
1	B	156	ALA
1	B	366	ALA
1	D	156	ALA
1	A	263	LYS
1	C	263	LYS
1	B	263	LYS
1	B	367	MET
1	D	263	LYS
1	D	366	ALA
1	D	372	SER

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	392/422 (93%)	361 (92%)	31 (8%)	12	31
1	B	390/422 (92%)	363 (93%)	27 (7%)	15	38
1	C	393/422 (93%)	368 (94%)	25 (6%)	17	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	395/422 (94%)	373 (94%)	22 (6%)	21 47
All	All	1570/1688 (93%)	1465 (93%)	105 (7%)	16 39

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	44	ARG
1	A	100	ASP
1	A	133	LEU
1	A	138	ARG
1	A	154	ARG
1	A	169	LEU
1	A	197	ARG
1	A	208	HIS
1	A	235	ARG
1	A	240	ASP
1	A	241	GLU
1	A	243	GLU
1	A	255	SER
1	A	260	SER
1	A	263	LYS
1	A	292	THR
1	A	317	VAL
1	A	339	TYR
1	A	359	ARG
1	A	367	MET
1	A	372	SER
1	A	395	ASP
1	A	398	ARG
1	A	422	SER
1	A	426	SER
1	A	428	VAL
1	A	434	MET
1	A	446	THR
1	A	448	GLN
1	A	522	LEU
1	C	26	VAL
1	C	93	GLN
1	C	103	ARG
1	C	169	LEU
1	C	197	ARG

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Mol	Chain	Res	Type
1	C	206	SER
1	C	208	HIS
1	C	235	ARG
1	C	243	GLU
1	C	247	LYS
1	C	255	SER
1	C	260	SER
1	C	267	ARG
1	C	292	THR
1	C	317	VAL
1	C	339	TYR
1	C	359	ARG
1	C	367	MET
1	C	369	VAL
1	C	398	ARG
1	C	402	ARG
1	C	422	SER
1	C	426	SER
1	C	434	MET
1	C	446	THR
1	B	7	GLU
1	B	26	VAL
1	B	100	ASP
1	B	169	LEU
1	B	197	ARG
1	B	206	SER
1	B	235	ARG
1	B	240	ASP
1	B	241	GLU
1	B	243	GLU
1	B	247	LYS
1	B	255	SER
1	B	260	SER
1	B	271	ARG
1	B	292	THR
1	B	299	GLU
1	B	317	VAL
1	B	339	TYR
1	B	359	ARG
1	B	395	ASP
1	B	398	ARG
1	B	418	ARG

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Mol	Chain	Res	Type
1	B	422	SER
1	B	426	SER
1	B	434	MET
1	B	446	THR
1	B	448	GLN
1	D	7	GLU
1	D	26	VAL
1	D	100	ASP
1	D	169	LEU
1	D	197	ARG
1	D	206	SER
1	D	208	HIS
1	D	235	ARG
1	D	240	ASP
1	D	241	GLU
1	D	243	GLU
1	D	255	SER
1	D	260	SER
1	D	263	LYS
1	D	319	THR
1	D	339	TYR
1	D	359	ARG
1	D	395	ASP
1	D	422	SER
1	D	426	SER
1	D	446	THR
1	D	448	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	C	113	ASN
1	C	444	ASN
1	C	448	GLN
1	B	113	ASN
1	B	124	ASN
1	B	401	GLN
1	D	113	ASN
1	D	448	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	486/523 (92%)	-0.20	12 (2%)	57	54	18, 33, 79, 119	0
1	B	483/523 (92%)	-0.10	26 (5%)	25	21	18, 34, 82, 108	0
1	C	487/523 (93%)	-0.15	26 (5%)	26	22	17, 31, 75, 97	0
1	D	489/523 (93%)	-0.20	10 (2%)	65	62	18, 33, 85, 121	0
All	All	1945/2092 (92%)	-0.16	74 (3%)	40	35	17, 33, 81, 121	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	LEU	5.3
1	C	161	THR	4.6
1	B	159	THR	4.5
1	B	161	THR	4.4
1	B	158	THR	4.3
1	B	163	THR	3.9
1	C	160	GLY	3.8
1	A	184	ALA	3.5
1	B	160	GLY	3.4
1	A	523	SER	3.4
1	C	156	ALA	3.2
1	C	168	SER	3.2
1	B	170	PRO	3.1
1	B	157	LEU	3.1
1	A	192	GLU	3.1
1	C	153	ALA	3.1
1	D	192	GLU	3.0
1	D	523	SER	2.9
1	C	44	ARG	2.9
1	B	168	SER	2.9
1	C	42	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	183	ILE	2.9
1	D	161	THR	2.9
1	B	164	LEU	2.8
1	C	41	ASP	2.7
1	D	170	PRO	2.7
1	B	523	SER	2.7
1	C	163	THR	2.7
1	B	42	GLU	2.7
1	A	168	SER	2.6
1	C	162	ALA	2.6
1	B	268	VAL	2.6
1	C	159	THR	2.6
1	C	523	SER	2.6
1	C	164	LEU	2.6
1	D	372	SER	2.6
1	A	179	VAL	2.5
1	A	188	ARG	2.5
1	D	169	LEU	2.5
1	B	167	ALA	2.5
1	B	260	SER	2.5
1	C	236	PHE	2.5
1	C	263	LYS	2.5
1	C	155	GLU	2.5
1	C	166	THR	2.5
1	B	154	ARG	2.5
1	A	170	PRO	2.5
1	B	178	ASP	2.4
1	B	263	LYS	2.4
1	B	169	LEU	2.4
1	B	41	ASP	2.4
1	C	170	PRO	2.4
1	D	166	THR	2.4
1	D	181	GLY	2.3
1	C	158	THR	2.2
1	A	236	PHE	2.2
1	B	179	VAL	2.2
1	B	166	THR	2.2
1	B	265	THR	2.2
1	B	151	ASP	2.2
1	D	184	ALA	2.2
1	A	161	THR	2.2
1	A	178	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	2.1
1	B	44	ARG	2.1
1	B	155	GLU	2.1
1	B	153	ALA	2.1
1	C	182	VAL	2.1
1	C	183	ILE	2.1
1	D	195	ALA	2.1
1	C	268	VAL	2.1
1	C	261	LEU	2.0
1	C	151	ASP	2.0
1	C	365	PRO	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.