Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:53 AM GMT

PDB ID	:	3K3W
Title	:	Thermostable Penicillin G acylase from Alcaligenes faecalis in orthorhombic form
Authors	:	Varshney, N.K.; Kumar, R.S.; Ignatova, Z.; Dodson, E.; Suresh, C.G.
Deposited on	:	2009-10-05
Resolution	:	3.31 Å(reported)

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

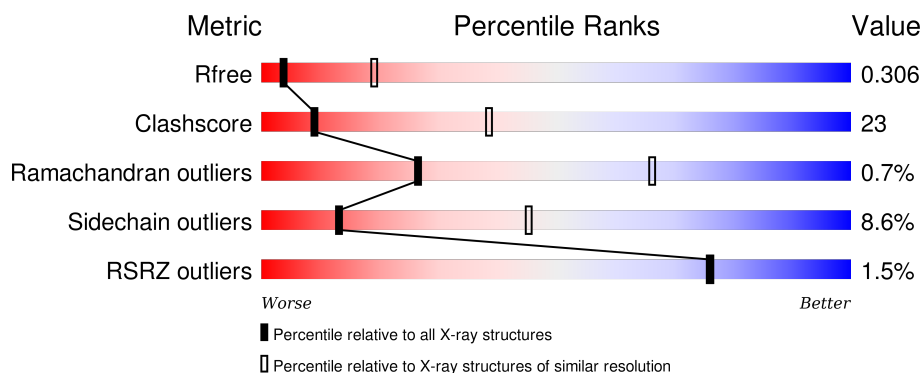|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.31 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	Percentile Ranks	Value
Rfree		0.306
Clashscore		23
Ramachandran outliers		0.7%
Sidechain outliers		8.6%
RSRZ outliers		1.5%

Worse				*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	196	2% 70% 27% •
2	B	551	% 66% 29% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6011 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 Penicillin G acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	2	0	0
			1573	996	271	299	7			

- Molecule 2 is a protein called Penicillin G acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	551	Total	C	N	O	S	39	0	0
			4427	2797	778	831	21			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	6	Total	O	0	0
			6	6		

3 Residue-property plots ⓘ

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: Penicillin G acylase
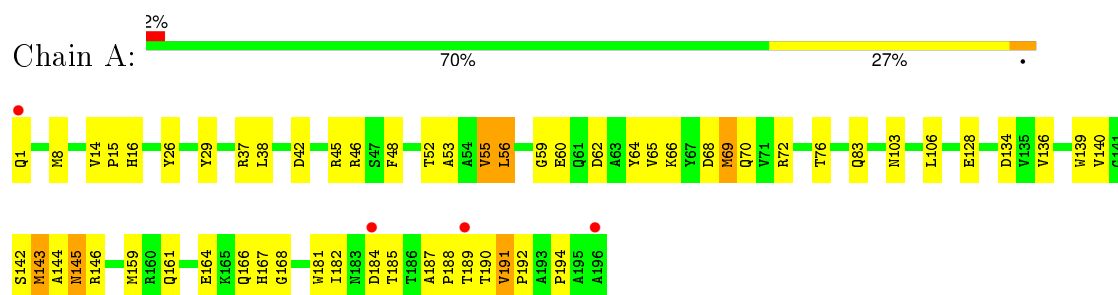
- Molecule 2: Penicillin G acylase
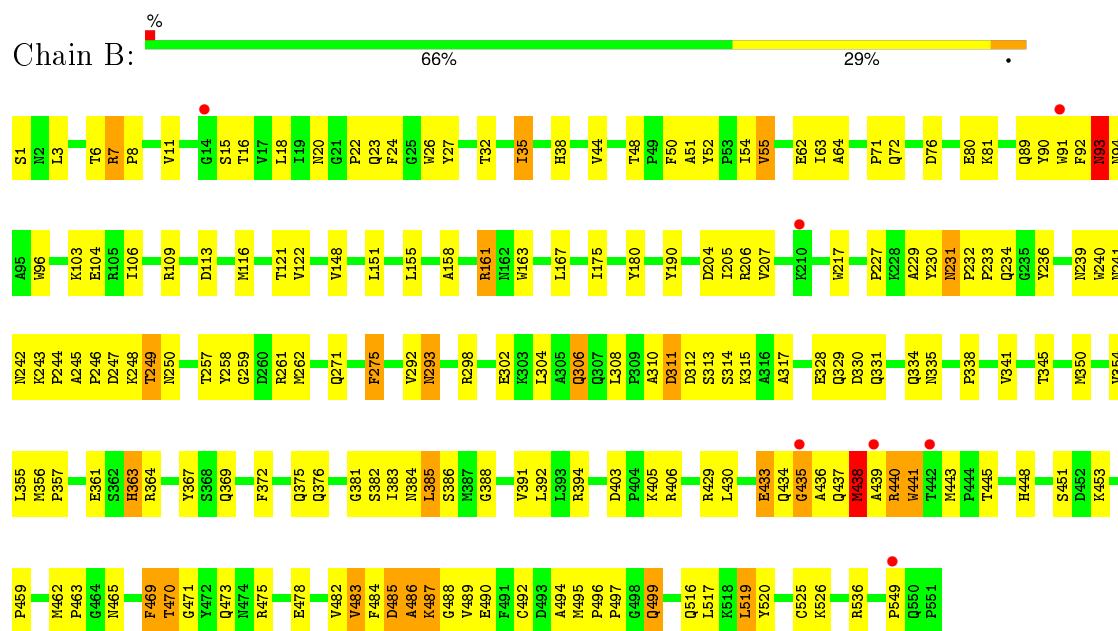
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	72.93Å 86.02Å 260.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.82 – 3.31	Depositor
	46.82 – 3.31	EDS
% Data completeness	99.7 (46.82-3.31)	Depositor
(in resolution range)	99.6 (46.82-3.31)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.06 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.281 , 0.315	Depositor
	0.273 , 0.306	DCC
R_{free} test set	612 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 32.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 12602 reflections	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	6011	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.31	0/1612	0.45	0/2190
2	B	0.31	0/4554	0.45	0/6192
All	All	0.31	0/6166	0.45	0/8382

There are no bond length outliers.

There are no bond angle outliers.

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	1573	0	1505	83	0
2	B	4427	0	4212	227	0
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	6	0	0	0	0
All	All	6011	0	5717	270	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 23.

All (270) 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:B:338:PRO:HB3	2:B:441:TRP:HB2	1.27	1.09
1:A:140:VAL:O	1:A:145:ASN:HB2	1.53	1.09
2:B:161:ARG:HG2	2:B:161:ARG:HH11	1.20	1.06
2:B:311:ASP:O	2:B:312:ASP:OD1	1.73	1.06
2:B:436:ALA:HA	2:B:441:TRP:CH2	1.92	1.02
2:B:436:ALA:HA	2:B:441:TRP:HH2	1.18	1.01
1:A:139:TRP:CE2	1:A:143:MET:HG3	1.99	0.97
1:A:139:TRP:NE1	1:A:143:MET:HG3	1.83	0.94
2:B:434:GLN:CG	2:B:441:TRP:CZ3	2.52	0.93
2:B:436:ALA:CA	2:B:441:TRP:CH2	2.51	0.93
2:B:121:THR:HG22	2:B:122:VAL:H	1.34	0.91
2:B:436:ALA:CA	2:B:441:TRP:HH2	1.83	0.90
2:B:328:GLU:HG2	2:B:328:GLU:O	1.74	0.87
1:A:55:VAL:O	2:B:109:ARG:HD3	1.75	0.87
2:B:434:GLN:HG2	2:B:441:TRP:CE3	2.10	0.86
2:B:240:TRP:CD1	2:B:261:ARG:HD2	2.14	0.83
2:B:438:MET:HA	2:B:441:TRP:CD1	2.14	0.83
2:B:499:GLN:HG3	2:B:499:GLN:O	1.76	0.82
1:A:59:GLY:CA	1:A:60:GLU:C	2.47	0.82
2:B:487:LYS:NZ	2:B:487:LYS:CB	2.41	0.82
2:B:121:THR:HG22	2:B:122:VAL:N	1.94	0.81
2:B:487:LYS:NZ	2:B:487:LYS:HB3	1.96	0.80
2:B:338:PRO:CB	2:B:441:TRP:HB2	2.11	0.80
2:B:161:ARG:NH1	2:B:161:ARG:HG2	1.94	0.80
2:B:484:PHE:CE1	2:B:489:VAL:HG23	2.18	0.79
2:B:434:GLN:HG2	2:B:441:TRP:CZ3	2.18	0.78
2:B:161:ARG:CG	2:B:161:ARG:HH11	1.96	0.78
2:B:494:ALA:HB1	2:B:519:LEU:HD21	1.65	0.77
2:B:484:PHE:CE1	2:B:489:VAL:CG2	2.68	0.77
1:A:191:VAL:HG13	1:A:192:PRO:HD3	1.67	0.76
2:B:497:PRO:O	2:B:516:GLN:HB2	1.86	0.76
2:B:434:GLN:HG3	2:B:441:TRP:HZ3	1.49	0.76
1:A:68:ASP:O	1:A:72:ARG:HG2	1.85	0.76
1:A:65:VAL:O	1:A:69:MET:HG3	1.86	0.75
2:B:433:GLU:HG2	2:B:434:GLN:H	1.51	0.75
2:B:483:VAL:HG23	2:B:490:GLU:HB3	1.69	0.74
1:A:192:PRO:HG2	2:B:244:PRO:O	1.88	0.74
2:B:436:ALA:N	2:B:441:TRP:CH2	2.57	0.73
2:B:245:ALA:HB1	2:B:246:PRO:HD2	1.69	0.73
2:B:496:PRO:HG3	2:B:520:TYR:CG	2.24	0.72
2:B:434:GLN:HG3	2:B:441:TRP:CZ3	2.23	0.72
2:B:330:ASP:HB2	2:B:445:THR:OG1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HA	2:B:499:GLN:NE2	2.05	0.72
2:B:487:LYS:CB	2:B:487:LYS:HZ2	2.04	0.71
1:A:139:TRP:NE1	1:A:143:MET:CG	2.54	0.70
2:B:310:ALA:HA	2:B:315:LYS:HD3	1.72	0.70
2:B:3:LEU:HD12	2:B:20:ASN:HB2	1.74	0.70
2:B:434:GLN:CG	2:B:441:TRP:HZ3	2.01	0.70
2:B:338:PRO:HB3	2:B:441:TRP:CB	2.17	0.69
2:B:71:PRO:HG2	2:B:244:PRO:HG3	1.75	0.68
2:B:7:ARG:HH22	2:B:231:ASN:ND2	1.92	0.68
2:B:494:ALA:O	2:B:496:PRO:HD3	1.94	0.68
2:B:441:TRP:HA	2:B:441:TRP:CE3	2.29	0.68
1:A:59:GLY:HA2	1:A:62:ASP:N	2.09	0.68
2:B:383:ILE:HG22	2:B:384:ASN:N	2.09	0.68
2:B:430:LEU:O	2:B:434:GLN:HB3	1.93	0.67
2:B:90:TYR:O	2:B:96:TRP:HE3	1.77	0.67
2:B:487:LYS:HZ2	2:B:487:LYS:HB3	1.59	0.67
2:B:121:THR:CG2	2:B:122:VAL:H	2.06	0.67
2:B:484:PHE:HE1	2:B:489:VAL:CG2	2.06	0.67
1:A:59:GLY:HA3	1:A:60:GLU:C	2.15	0.67
2:B:385:LEU:HD12	2:B:385:LEU:N	2.09	0.67
1:A:192:PRO:HB3	2:B:229:ALA:HB2	1.77	0.66
1:A:190:THR:HG22	2:B:243:LYS:HB3	1.78	0.66
2:B:441:TRP:HA	2:B:441:TRP:HE3	1.60	0.66
2:B:90:TYR:CZ	2:B:121:THR:HG23	2.31	0.66
2:B:242:ASN:ND2	2:B:262:MET:SD	2.69	0.66
1:A:37:ARG:HH21	2:B:499:GLN:HA	1.60	0.66
2:B:80:GLU:OE2	2:B:121:THR:HG21	1.96	0.66
1:A:139:TRP:O	1:A:143:MET:HB2	1.97	0.65
1:A:15:PRO:HD2	2:B:499:GLN:NE2	2.11	0.65
1:A:59:GLY:HA2	1:A:60:GLU:C	2.18	0.64
2:B:497:PRO:HG3	2:B:517:LEU:HD12	1.80	0.64
2:B:485:ASP:O	2:B:487:LYS:N	2.30	0.64
1:A:142:SER:CB	2:B:50:PHE:CE2	2.80	0.64
2:B:434:GLN:O	2:B:436:ALA:N	2.30	0.64
2:B:7:ARG:HH22	2:B:231:ASN:CG	2.01	0.64
2:B:497:PRO:O	2:B:516:GLN:CB	2.47	0.63
1:A:142:SER:HB2	2:B:50:PHE:HE2	1.63	0.63
2:B:18:LEU:O	2:B:18:LEU:HD23	1.98	0.62
1:A:166:GLN:NE2	1:A:167:HIS:CE1	2.67	0.62
1:A:185:THR:O	1:A:188:PRO:HD2	1.99	0.62
2:B:240:TRP:NE1	2:B:261:ARG:HD2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:PHE:HB2	2:B:52:TYR:CE1	2.35	0.62
1:A:42:ASP:O	1:A:46:ARG:HG3	1.99	0.62
1:A:15:PRO:HD2	2:B:499:GLN:HE22	1.64	0.62
1:A:69:MET:HG2	2:B:106:ILE:HD13	1.81	0.62
2:B:241:ASN:CB	2:B:261:ARG:NH2	2.63	0.61
2:B:448:HIS:CB	2:B:469:PHE:HB2	2.30	0.61
2:B:384:ASN:OD1	2:B:385:LEU:N	2.30	0.61
1:A:59:GLY:HA3	1:A:60:GLU:O	1.99	0.61
2:B:437:GLN:O	2:B:440:ARG:N	2.30	0.61
2:B:448:HIS:HB3	2:B:469:PHE:HB2	1.82	0.61
1:A:45:ARG:HG3	1:A:134:ASP:HB3	1.82	0.60
1:A:166:GLN:HE21	1:A:167:HIS:CE1	2.19	0.60
1:A:139:TRP:O	1:A:143:MET:N	2.35	0.60
2:B:261:ARG:NH1	2:B:382:SER:HB2	2.17	0.60
2:B:26:TRP:CE2	2:B:448:HIS:HE1	2.19	0.60
2:B:433:GLU:HG2	2:B:434:GLN:N	2.16	0.60
2:B:487:LYS:HZ3	2:B:487:LYS:HB3	1.67	0.59
1:A:181:TRP:CD1	1:A:184:ASP:HA	2.37	0.59
2:B:483:VAL:CG2	2:B:490:GLU:HB3	2.32	0.59
1:A:136:VAL:O	1:A:140:VAL:HG13	2.02	0.59
1:A:164:GLU:HA	1:A:168:GLY:HA3	1.84	0.59
1:A:48:PHE:CZ	1:A:142:SER:HB3	2.37	0.59
2:B:93:ASN:C	2:B:93:ASN:OD1	2.41	0.59
2:B:240:TRP:O	2:B:241:ASN:HB2	2.02	0.59
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.37	0.59
2:B:90:TYR:HE1	2:B:92:PHE:HB2	1.67	0.58
2:B:494:ALA:HB1	2:B:519:LEU:CD2	2.33	0.58
2:B:350:MET:O	2:B:354:VAL:HB	2.04	0.58
1:A:142:SER:CB	2:B:50:PHE:HE2	2.17	0.57
2:B:361:GLU:HA	2:B:364:ARG:HB2	1.86	0.57
1:A:1:GLN:CD	2:B:549:PRO:HG2	2.24	0.57
1:A:159:MET:HA	2:B:363:HIS:HE1	1.70	0.57
2:B:328:GLU:CG	2:B:328:GLU:O	2.49	0.56
1:A:144:ALA:CB	2:B:175:ILE:HG21	2.36	0.56
2:B:496:PRO:HB3	2:B:516:GLN:O	2.04	0.56
2:B:76:ASP:HB2	2:B:217:TRP:HZ2	1.71	0.56
2:B:453:LYS:HB3	2:B:459:PRO:HA	1.87	0.55
1:A:142:SER:OG	2:B:50:PHE:CD2	2.52	0.55
1:A:139:TRP:O	1:A:143:MET:CB	2.55	0.55
1:A:187:ALA:N	1:A:188:PRO:CD	2.69	0.55
2:B:485:ASP:O	2:B:488:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:GLY:O	2:B:436:ALA:HB3	2.07	0.54
1:A:192:PRO:CG	2:B:244:PRO:O	2.55	0.54
2:B:292:VAL:CG1	2:B:385:LEU:HD11	2.38	0.54
2:B:363:HIS:N	2:B:363:HIS:CD2	2.75	0.54
2:B:384:ASN:OD1	2:B:385:LEU:HD12	2.07	0.54
1:A:55:VAL:HG23	1:A:56:LEU:HG	1.90	0.54
2:B:23:GLN:OE1	2:B:382:SER:HB3	2.08	0.53
2:B:403:ASP:HB3	2:B:406:ARG:HB3	1.90	0.53
2:B:330:ASP:CB	2:B:445:THR:OG1	2.55	0.53
2:B:489:VAL:HG22	2:B:490:GLU:N	2.24	0.53
1:A:14:VAL:HA	2:B:499:GLN:HE21	1.71	0.53
1:A:16:HIS:HD2	2:B:38:HIS:CE1	2.25	0.53
2:B:345:THR:HG21	2:B:430:LEU:HD11	1.90	0.53
2:B:434:GLN:CG	2:B:441:TRP:CE3	2.81	0.53
1:A:139:TRP:CE2	1:A:143:MET:CG	2.85	0.52
1:A:53:ALA:HA	1:A:56:LEU:O	2.10	0.52
2:B:241:ASN:HB2	2:B:261:ARG:NH2	2.24	0.52
2:B:487:LYS:CB	2:B:487:LYS:HZ3	2.22	0.52
2:B:245:ALA:O	2:B:248:LYS:HB2	2.10	0.52
1:A:16:HIS:HD2	2:B:38:HIS:HE1	1.58	0.52
1:A:16:HIS:CD2	2:B:38:HIS:HE1	2.27	0.52
1:A:72:ARG:HH11	2:B:104:GLU:HG3	1.76	0.51
2:B:3:LEU:HD12	2:B:20:ASN:CB	2.40	0.51
2:B:54:ILE:HA	2:B:155:LEU:HD23	1.92	0.51
2:B:26:TRP:CD2	2:B:448:HIS:HE1	2.29	0.51
1:A:45:ARG:HH22	1:A:128:GLU:HB2	1.75	0.51
2:B:470:THR:N	2:B:471:GLY:HA3	2.26	0.51
2:B:48:THR:HB	2:B:55:VAL:HA	1.93	0.51
1:A:15:PRO:CD	2:B:499:GLN:NE2	2.73	0.51
1:A:184:ASP:CG	1:A:188:PRO:HG2	2.32	0.50
1:A:182:ILE:O	2:B:249:THR:HG22	2.10	0.50
2:B:204:ASP:HB3	2:B:207:VAL:HG22	1.91	0.50
2:B:434:GLN:CB	2:B:441:TRP:CZ3	2.94	0.50
1:A:190:THR:HB	1:A:192:PRO:HD2	1.92	0.50
2:B:7:ARG:NH2	2:B:231:ASN:OD1	2.45	0.50
1:A:159:MET:CA	2:B:363:HIS:HE1	2.24	0.50
2:B:434:GLN:HB3	2:B:441:TRP:CZ3	2.47	0.50
2:B:495:MET:CG	2:B:495:MET:O	2.59	0.50
2:B:317:ALA:HA	2:B:438:MET:HE1	1.94	0.49
1:A:65:VAL:O	1:A:69:MET:CG	2.59	0.49
1:A:188:PRO:HG3	2:B:257:THR:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:PRO:HB2	2:B:234:GLN:HG2	1.93	0.49
2:B:496:PRO:HG3	2:B:520:TYR:CD1	2.48	0.49
1:A:191:VAL:HG11	2:B:239:ASN:HD22	1.78	0.49
2:B:499:GLN:CG	2:B:499:GLN:O	2.55	0.49
2:B:7:ARG:HB2	2:B:8:PRO:HD2	1.95	0.48
2:B:11:VAL:HG11	2:B:15:SER:O	2.13	0.48
1:A:62:ASP:O	1:A:66:LYS:HG3	2.13	0.48
2:B:485:ASP:O	2:B:486:ALA:C	2.52	0.48
2:B:485:ASP:C	2:B:487:LYS:N	2.66	0.48
1:A:144:ALA:HB2	2:B:175:ILE:HG21	1.95	0.48
1:A:29:TYR:CD1	2:B:35:ILE:HD12	2.49	0.48
1:A:59:GLY:HA2	1:A:62:ASP:H	1.76	0.48
2:B:484:PHE:CD1	2:B:489:VAL:HG23	2.47	0.48
2:B:26:TRP:HZ3	2:B:381:GLY:HA2	1.78	0.48
2:B:356:MET:CB	2:B:357:PRO:HD3	2.44	0.48
2:B:433:GLU:CG	2:B:434:GLN:N	2.77	0.47
2:B:434:GLN:C	2:B:436:ALA:N	2.67	0.47
2:B:436:ALA:N	2:B:441:TRP:HH2	2.00	0.47
2:B:275:PHE:CD2	2:B:275:PHE:N	2.82	0.47
2:B:90:TYR:CE2	2:B:121:THR:HG23	2.49	0.47
2:B:230:TYR:O	2:B:231:ASN:O	2.32	0.47
2:B:448:HIS:CD2	2:B:473:GLN:H	2.33	0.47
2:B:497:PRO:O	2:B:516:GLN:CA	2.62	0.47
2:B:356:MET:HB2	2:B:357:PRO:HD3	1.97	0.47
2:B:91:TRP:CD1	2:B:91:TRP:C	2.89	0.47
2:B:227:PRO:HG3	2:B:248:LYS:HE3	1.96	0.46
2:B:90:TYR:CE1	2:B:92:PHE:HB2	2.48	0.46
2:B:330:ASP:HB3	2:B:445:THR:CG2	2.45	0.46
1:A:194:PRO:HB3	2:B:246:PRO:HB3	1.97	0.46
2:B:249:THR:HG22	2:B:250:ASN:H	1.80	0.46
2:B:64:ALA:HB2	2:B:482:VAL:HG11	1.96	0.46
1:A:182:ILE:HG22	2:B:205:ILE:HG22	1.98	0.46
2:B:227:PRO:HB3	2:B:245:ALA:HB2	1.98	0.46
2:B:257:THR:HG23	2:B:259:GLY:H	1.81	0.46
2:B:89:GLN:NE2	2:B:96:TRP:HB3	2.30	0.46
1:A:52:THR:O	1:A:56:LEU:HD12	2.16	0.46
2:B:311:ASP:CG	2:B:312:ASP:N	2.70	0.45
2:B:241:ASN:HB2	2:B:261:ARG:CZ	2.47	0.45
2:B:475:ARG:NH1	2:B:520:TYR:O	2.50	0.45
1:A:69:MET:HB3	2:B:116:MET:SD	2.56	0.45
2:B:354:VAL:HG11	2:B:392:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:THR:HG22	2:B:429:ARG:HH21	1.82	0.45
2:B:341:VAL:HG22	2:B:443:MET:HG2	1.98	0.45
2:B:161:ARG:CG	2:B:161:ARG:NH1	2.65	0.45
2:B:497:PRO:O	2:B:516:GLN:N	2.50	0.45
2:B:241:ASN:OD1	2:B:261:ARG:NH2	2.50	0.44
2:B:367:TYR:O	2:B:388:GLY:HA3	2.17	0.44
2:B:163:TRP:CE2	2:B:167:LEU:HD11	2.52	0.44
2:B:121:THR:CG2	2:B:122:VAL:N	2.64	0.44
2:B:355:LEU:CD1	2:B:388:GLY:HA2	2.48	0.44
2:B:485:ASP:HB2	2:B:487:LYS:HG3	1.99	0.44
1:A:103:ASN:HA	1:A:106:LEU:HB3	1.99	0.44
1:A:59:GLY:CA	1:A:60:GLU:O	2.61	0.44
2:B:3:LEU:HD13	2:B:180:TYR:CD2	2.53	0.44
1:A:139:TRP:CZ2	1:A:143:MET:HG3	2.49	0.44
2:B:22:PRO:HD2	2:B:478:GLU:O	2.18	0.44
2:B:302:GLU:O	2:B:306:GLN:HG3	2.18	0.44
1:A:188:PRO:HA	2:B:258:TYR:HA	2.00	0.44
1:A:187:ALA:N	1:A:188:PRO:HD2	2.32	0.43
1:A:192:PRO:HG3	2:B:190:TYR:CE2	2.52	0.43
2:B:292:VAL:HG12	2:B:385:LEU:HD11	2.00	0.43
2:B:54:ILE:HG12	2:B:155:LEU:HB2	2.00	0.43
2:B:293:ASN:HB3	2:B:385:LEU:HD23	2.01	0.43
2:B:350:MET:O	2:B:354:VAL:CG2	2.66	0.43
2:B:27:TYR:HD1	2:B:451:SER:HB2	1.84	0.43
2:B:62:GLU:O	2:B:63:ILE:HG13	2.19	0.43
2:B:54:ILE:HG23	2:B:155:LEU:HA	2.00	0.43
1:A:15:PRO:HG2	2:B:35:ILE:HG13	2.01	0.42
2:B:487:LYS:HZ2	2:B:487:LYS:HB2	1.83	0.42
2:B:448:HIS:HD2	2:B:473:GLN:H	1.67	0.42
2:B:470:THR:H	2:B:471:GLY:HA3	1.84	0.42
1:A:72:ARG:HH11	2:B:104:GLU:CG	2.32	0.42
2:B:355:LEU:HD21	2:B:391:VAL:HG11	2.00	0.42
1:A:26:TYR:HA	1:A:29:TYR:HB3	2.02	0.42
2:B:330:ASP:HA	2:B:335:ASN:HA	2.02	0.42
2:B:234:GLN:HB2	2:B:236:TYR:CE2	2.55	0.42
1:A:8:MET:O	1:A:15:PRO:HA	2.20	0.42
2:B:50:PHE:O	2:B:51:ALA:C	2.57	0.42
2:B:93:ASN:HA	2:B:94:ASN:HA	1.49	0.42
2:B:434:GLN:O	2:B:435:GLY:C	2.56	0.42
2:B:470:THR:HG23	2:B:471:GLY:HA3	2.02	0.42
2:B:304:LEU:O	2:B:308:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:SER:O	2:B:314:SER:HB2	2.19	0.42
2:B:375:GLN:HG3	2:B:376:GLN:N	2.35	0.42
2:B:525:CYS:SG	2:B:526:LYS:N	2.92	0.42
1:A:142:SER:OG	2:B:50:PHE:CE2	2.67	0.41
2:B:76:ASP:HB2	2:B:217:TRP:CZ2	2.53	0.41
2:B:356:MET:N	2:B:357:PRO:CD	2.83	0.41
2:B:462:MET:HA	2:B:463:PRO:HD3	1.91	0.41
2:B:1:SER:N	2:B:23:GLN:OE1	2.51	0.41
2:B:232:PRO:HA	2:B:233:PRO:HD3	1.93	0.41
2:B:246:PRO:HG2	2:B:247:ASP:H	1.85	0.41
2:B:436:ALA:HA	2:B:441:TRP:CZ2	2.50	0.41
2:B:494:ALA:CB	2:B:519:LEU:HD21	2.41	0.41
2:B:245:ALA:CB	2:B:246:PRO:HD2	2.40	0.41
1:A:139:TRP:HE3	1:A:140:VAL:HG12	1.86	0.41
2:B:7:ARG:HB2	2:B:8:PRO:CD	2.51	0.41
1:A:144:ALA:HB1	2:B:175:ILE:HG21	2.02	0.41
2:B:437:GLN:O	2:B:439:ALA:N	2.55	0.40
2:B:331:GLN:N	2:B:334:GLN:O	2.47	0.40
1:A:8:MET:SD	2:B:536:ARG:NH1	2.84	0.40
2:B:484:PHE:HE1	2:B:489:VAL:HG21	1.83	0.40
1:A:56:LEU:HD13	1:A:64:TYR:CE2	2.56	0.40
2:B:44:VAL:HG11	2:B:158:ALA:HB1	2.03	0.40
1:A:83:GLN:HE21	2:B:148:VAL:HG22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
2	B	549/551 (100%)	500 (91%)	44 (8%)	5 (1%)	21	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	743/747 (100%)	686 (92%)	52 (7%)	5 (1%)	26　66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	435	GLY
2	B	486	ALA
2	B	93	ASN
2	B	231	ASN
2	B	438	MET

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	164/164 (100%)	152 (93%)	12 (7%)	17　53
2	B	466/466 (100%)	424 (91%)	42 (9%)	12　42
All	All	630/630 (100%)	576 (91%)	54 (9%)	13　45

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	55	VAL
1	A	56	LEU
1	A	69	MET
1	A	70	GLN
1	A	76	THR
1	A	143	MET
1	A	145	ASN
1	A	146	ARG
1	A	161	GLN
1	A	189	THR
1	A	191	VAL
2	B	6	THR

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Mol	Chain	Res	Type
2	B	7	ARG
2	B	16	THR
2	B	32	THR
2	B	35	ILE
2	B	55	VAL
2	B	72	GLN
2	B	81	LYS
2	B	93	ASN
2	B	103	LYS
2	B	113	ASP
2	B	151	LEU
2	B	161	ARG
2	B	206	ARG
2	B	249	THR
2	B	271	GLN
2	B	275	PHE
2	B	293	ASN
2	B	298	ARG
2	B	306	GLN
2	B	311	ASP
2	B	329	GLN
2	B	363	HIS
2	B	369	GLN
2	B	372	PHE
2	B	385	LEU
2	B	386	SER
2	B	394	ARG
2	B	405	LYS
2	B	433	GLU
2	B	438	MET
2	B	440	ARG
2	B	441	TRP
2	B	465	ASN
2	B	469	PHE
2	B	470	THR
2	B	483	VAL
2	B	485	ASP
2	B	487	LYS
2	B	492	CYS
2	B	499	GLN
2	B	519	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	73	GLN
1	A	83	GLN
1	A	151	ASN
1	A	166	GLN
1	A	167	HIS
2	B	38	HIS
2	B	169	GLN
2	B	307	GLN
2	B	329	GLN
2	B	335	ASN
2	B	363	HIS
2	B	379	ASN
2	B	425	ASN
2	B	448	HIS
2	B	465	ASN
2	B	474	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	196/196 (100%)	0.14	4 (2%)	68	67	21, 39, 55, 83	1 (0%)
2	B	549/551 (99%)	0.25	7 (1%)	79	79	25, 42, 60, 74	6 (1%)
All	All	745/747 (99%)	0.22	11 (1%)	76	76	21, 41, 59, 83	7 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ALA	4.0
2	B	439	ALA	3.7
1	A	184	ASP	3.0
2	B	91	TRP	2.8
1	A	189	THR	2.6
2	B	14	GLY	2.4
2	B	435	GLY	2.4
2	B	442	THR	2.3
1	A	1	GLN	2.2
2	B	210	LYS	2.1
2	B	549	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	B	552	1/1	0.90	0.09	-3.12	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.