Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 02:14 am BST

PDB ID	:	3BXW
Title	:	Crystal Structure of Stabilin-1 Interacting Chitinase-Like Protein, SI-CLP
Authors	:	Meng, G.; Green, T.J.
Deposited on	:	2008-01-15
Resolution	:	2.70 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.

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.
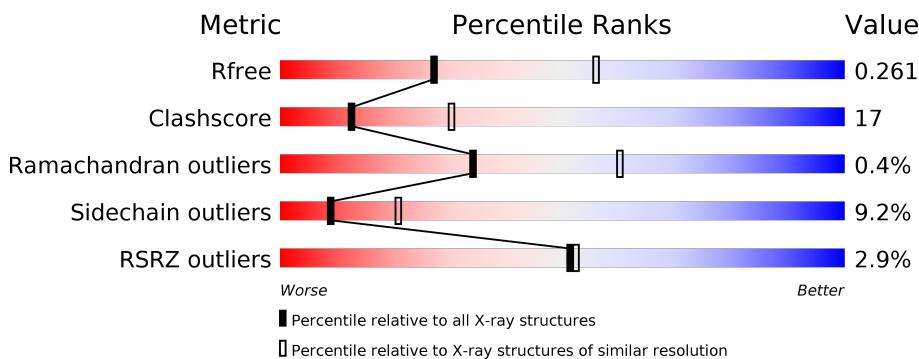
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	393	3% / 65% / 22% / · · / 8%
1	B	393	2% / 63% / 24% / 5% / 8%
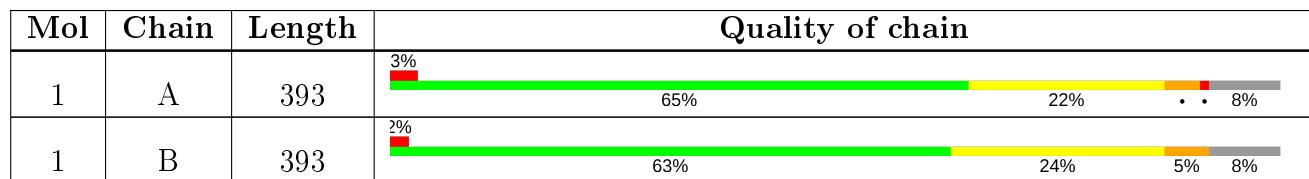
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	372	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5876 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 Chitinase domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	360	Total	C	N	O	S	0	0	0
			2923	1877	512	525	9			
1	A	360	Total	C	N	O	S	0	0	0
			2923	1876	512	526	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
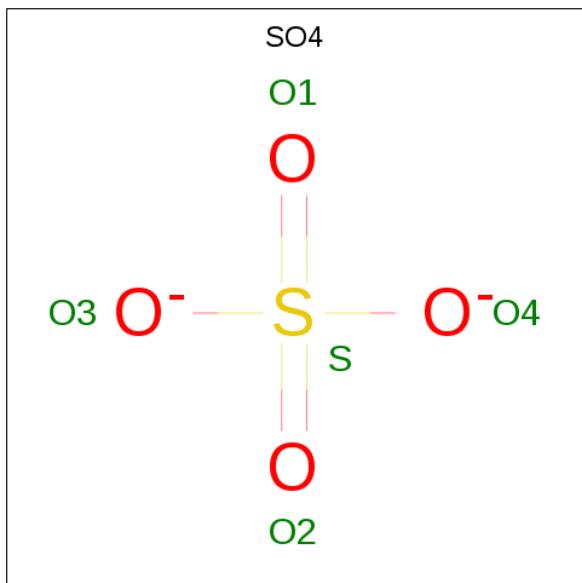
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	15	Total 15	O 15	0	0
3	A	5	Total 5	O 5	0	0

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 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: Chitinase domain-containing protein 1
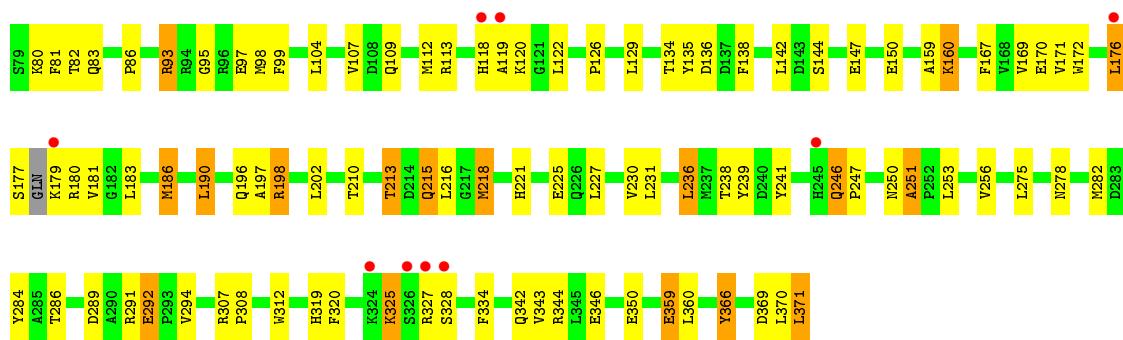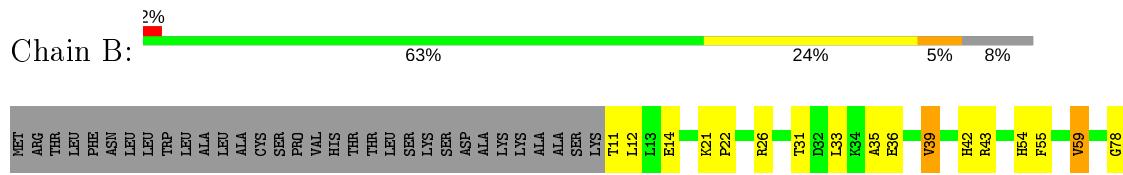
• Molecule 1: Chitinase domain-containing protein 1
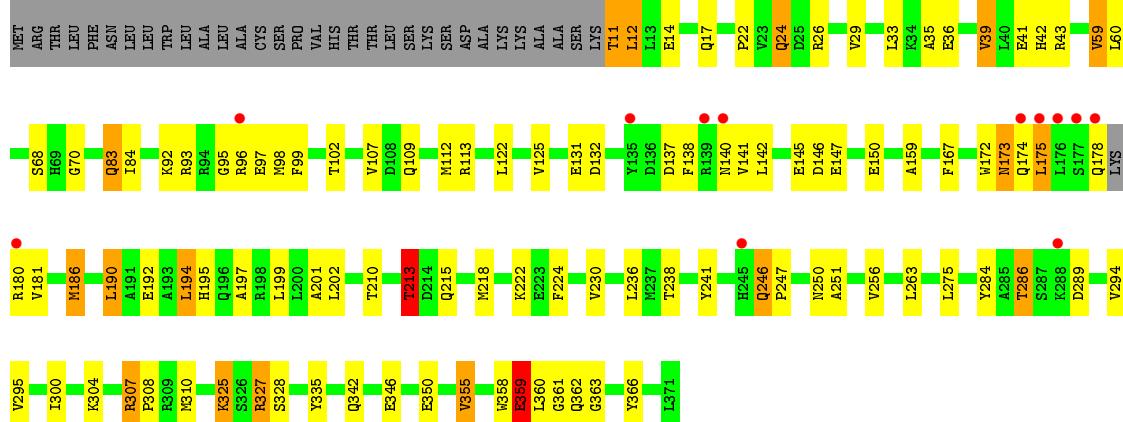
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.11Å 100.11Å 249.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 39.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.70) 100.0 (39.07-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$<I/\sigma(I)>$ [1]	1.97 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.253 0.229 , 0.261	Depositor DCC
R_{free} test set	2041 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.1	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5876	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4

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	0.45	0/2999	0.74	8/4064 (0.2%)
1	B	0.47	0/2999	0.84	8/4063 (0.2%)
All	All	0.46	0/5998	0.79	16/8127 (0.2%)

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
1	A	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	119	ALA	CB-CA-C	-21.86	77.31	110.10
1	B	120	LYS	N-CA-CB	-14.25	84.95	110.60
1	A	359	GLU	N-CA-CB	-11.72	89.51	110.60
1	B	176	LEU	N-CA-C	9.23	135.92	111.00
1	B	359	GLU	N-CA-CB	7.56	124.21	110.60
1	B	177	SER	N-CA-CB	-6.61	100.59	110.50
1	B	171	VAL	N-CA-CB	-6.21	97.83	111.50
1	A	358	TRP	C-N-CA	6.20	137.19	121.70
1	A	238	THR	N-CA-C	-5.87	95.15	111.00
1	A	251	ALA	N-CA-CB	-5.86	101.90	110.10
1	A	286	THR	CB-CA-C	-5.79	95.96	111.60
1	A	172	TRP	N-CA-C	5.74	126.50	111.00
1	B	170	GLU	CB-CA-C	-5.62	99.16	110.40
1	B	251	ALA	N-CA-CB	-5.53	102.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	THR	N-CA-CB	-5.31	100.21	110.30
1	A	172	TRP	CB-CA-C	-5.30	99.80	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	THR	Peptide
1	A	359	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2923	0	2890	99	0
1	B	2923	0	2896	95	0
2	B	10	0	0	2	0
3	A	5	0	0	0	0
3	B	15	0	0	0	0
All	All	5876	0	5786	194	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 17.

All (194) 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:12:LEU:N	1:A:12:LEU:HD23	1.57	1.12
1:A:11:THR:C	1:A:12:LEU:HD23	1.69	1.12
1:A:178:GLN:CD	1:A:218:MET:HE3	1.68	1.11
1:A:11:THR:O	1:A:12:LEU:HD23	1.64	0.97
1:A:178:GLN:CG	1:A:218:MET:HE3	1.97	0.94
1:B:370:LEU:O	1:B:371:LEU:HB2	1.64	0.94
1:A:12:LEU:N	1:A:12:LEU:CD2	2.32	0.91
1:A:327:ARG:NH1	1:A:327:ARG:HB3	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HH11	1:A:327:ARG:HB3	1.37	0.89
1:A:178:GLN:NE2	1:A:218:MET:HE3	1.89	0.86
1:A:11:THR:C	1:A:12:LEU:CD2	2.44	0.85
1:A:22:PRO:HB2	1:A:24:GLN:HE22	1.41	0.85
1:B:325:LYS:HE2	1:B:325:LYS:HA	1.58	0.85
1:A:24:GLN:H	1:A:24:GLN:HE21	1.24	0.83
1:B:134:THR:HG22	1:B:136:ASP:H	1.43	0.83
1:B:54:HIS:H	1:B:371:LEU:HG	1.44	0.83
1:A:12:LEU:HD12	1:A:36:GLU:HG3	1.63	0.81
1:A:11:THR:HB	1:A:12:LEU:HA	1.63	0.81
1:A:178:GLN:CD	1:A:218:MET:CE	2.50	0.80
1:A:24:GLN:H	1:A:24:GLN:NE2	1.79	0.80
1:A:11:THR:O	1:A:12:LEU:CD2	2.30	0.79
1:B:230:VAL:HG23	1:B:231:LEU:HD13	1.65	0.78
1:A:178:GLN:HA	1:A:180:ARG:HG2	1.65	0.78
1:B:176:LEU:HD22	1:B:176:LEU:H	1.50	0.77
1:A:109:GLN:HA	1:A:112:MET:HE3	1.66	0.75
1:B:256:VAL:HG13	1:B:275:LEU:HD11	1.70	0.73
1:B:282:MET:HE2	1:B:291:ARG:HD2	1.70	0.72
1:B:54:HIS:H	1:B:371:LEU:CG	2.02	0.72
1:A:210:THR:O	1:A:213:THR:HG22	1.90	0.72
1:B:172:TRP:O	1:B:176:LEU:HD23	1.90	0.72
1:A:178:GLN:HG2	1:A:218:MET:HE3	1.70	0.71
1:A:325:LYS:HG3	1:A:327:ARG:HH22	1.56	0.70
1:B:104:LEU:O	1:B:107:VAL:HG13	1.90	0.70
1:B:327:ARG:NH1	1:B:328:SER:HB2	2.06	0.70
1:B:213:THR:HG23	1:B:215:GLN:H	1.57	0.68
1:B:327:ARG:HH12	1:B:328:SER:HB2	1.56	0.68
1:B:215:GLN:HG2	1:B:216:LEU:N	2.08	0.68
1:B:97:GLU:O	1:B:150:GLU:HG2	1.94	0.68
1:B:54:HIS:H	1:B:371:LEU:CD2	2.07	0.67
1:A:138:PHE:CD2	1:A:175:LEU:HG	2.30	0.67
1:B:54:HIS:N	1:B:371:LEU:HG	2.09	0.67
1:B:227:LEU:HB3	1:B:231:LEU:HD22	1.77	0.66
1:B:11:THR:HB	1:B:307:ARG:HH22	1.61	0.65
1:A:210:THR:HB	1:A:213:THR:HG21	1.79	0.65
1:B:160:LYS:HE2	1:B:197:ALA:HB1	1.78	0.65
1:B:176:LEU:HB3	1:B:218:MET:HG2	1.79	0.64
1:B:93:ARG:HG2	1:B:99:PHE:CE1	2.32	0.64
1:A:22:PRO:HB2	1:A:24:GLN:NE2	2.09	0.64
1:A:190:LEU:HD22	1:A:194:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:THR:HG22	1:B:135:TYR:N	2.14	0.63
1:A:173:ASN:H	1:A:173:ASN:HD22	1.44	0.63
1:A:342:GLN:O	1:A:346:GLU:HG3	1.98	0.63
1:B:210:THR:HB	1:B:213:THR:HG21	1.80	0.63
1:B:12:LEU:HD13	1:B:39:VAL:HG11	1.82	0.62
1:A:178:GLN:NE2	1:A:218:MET:CE	2.63	0.61
1:A:194:LEU:HD23	1:A:201:ALA:HB2	1.82	0.61
1:A:308:PRO:HG2	1:A:310:MET:HE1	1.83	0.60
1:B:109:GLN:HA	1:B:112:MET:HE3	1.83	0.60
1:B:346:GLU:O	1:B:350:GLU:HG2	2.02	0.60
1:A:24:GLN:HE21	1:A:24:GLN:N	1.98	0.59
1:B:176:LEU:HD22	1:B:176:LEU:N	2.16	0.59
1:B:95:GLY:HA3	1:B:98:MET:CE	2.34	0.58
1:A:173:ASN:H	1:A:173:ASN:ND2	2.00	0.58
1:B:82:THR:HG22	1:B:83:GLN:CD	2.24	0.57
1:A:178:GLN:CA	1:A:180:ARG:HG2	2.32	0.57
1:A:308:PRO:HG2	1:A:310:MET:CE	2.35	0.57
1:A:178:GLN:HB3	1:A:180:ARG:HE	1.70	0.57
1:B:256:VAL:CG1	1:B:275:LEU:HD11	2.33	0.57
1:B:172:TRP:CZ3	1:B:183:LEU:HD12	2.40	0.57
1:B:36:GLU:HA	1:B:39:VAL:CG1	2.34	0.57
1:A:180:ARG:HD2	1:A:180:ARG:N	2.20	0.57
1:A:197:ALA:O	1:A:199:LEU:HD13	2.05	0.56
1:A:178:GLN:HG2	1:A:218:MET:CE	2.36	0.56
1:A:224:PHE:HB2	1:A:263:LEU:HD11	1.88	0.56
1:B:176:LEU:CB	1:B:218:MET:HG2	2.35	0.56
1:A:202:LEU:HD12	1:A:202:LEU:N	2.21	0.55
1:A:125:VAL:HG23	1:A:125:VAL:O	2.07	0.55
1:A:241:TYR:HB3	1:A:250:ASN:O	2.07	0.55
1:A:97:GLU:O	1:A:150:GLU:HG2	2.07	0.55
1:B:344:ARG:HH11	1:B:344:ARG:HG3	1.71	0.54
1:B:134:THR:HG22	1:B:136:ASP:N	2.19	0.54
1:B:230:VAL:HG23	1:B:231:LEU:CD1	2.35	0.54
1:B:134:THR:CG2	1:B:135:TYR:N	2.71	0.54
1:A:256:VAL:HG13	1:A:275:LEU:HD11	1.90	0.54
1:A:35:ALA:O	1:A:39:VAL:HG12	2.07	0.54
1:A:84:ILE:HG12	1:A:122:LEU:HD11	1.89	0.54
1:A:92:LYS:HD2	1:A:102:THR:HG21	1.88	0.54
1:B:210:THR:O	1:B:213:THR:HG22	2.08	0.53
1:B:213:THR:CG2	1:B:215:GLN:H	2.21	0.53
1:B:241:TYR:HB3	1:B:250:ASN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TYR:OH	1:A:363:GLY:HA2	2.09	0.53
1:A:256:VAL:CG1	1:A:275:LEU:HD11	2.39	0.53
1:B:159:ALA:HB2	1:B:167:PHE:CZ	2.44	0.53
1:B:236:LEU:HD22	1:B:238:THR:HG23	1.90	0.53
1:A:295:VAL:HG12	1:A:362:GLN:HG2	1.92	0.52
1:A:175:LEU:CD2	1:A:175:LEU:C	2.77	0.52
1:B:241:TYR:CB	1:B:250:ASN:O	2.57	0.52
1:B:82:THR:HG22	1:B:83:GLN:NE2	2.24	0.52
1:A:14:GLU:HG3	1:A:39:VAL:O	2.10	0.51
1:B:282:MET:HE3	1:B:282:MET:HA	1.93	0.51
1:B:59:VAL:HG22	1:B:81:PHE:CD1	2.46	0.50
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.77	0.50
1:B:36:GLU:H	1:B:36:GLU:CD	2.13	0.50
1:B:213:THR:HG23	1:B:215:GLN:N	2.26	0.50
1:B:35:ALA:O	1:B:39:VAL:HG12	2.11	0.50
1:A:59:VAL:HA	1:A:355:VAL:O	2.12	0.50
1:A:325:LYS:HE2	1:A:327:ARG:HH12	1.77	0.50
1:B:179:LYS:HB3	1:B:181:VAL:HG12	1.94	0.49
1:B:80:LYS:HB3	1:B:371:LEU:HD13	1.92	0.49
1:B:325:LYS:CE	1:B:325:LYS:HA	2.32	0.49
1:A:138:PHE:CE2	1:A:175:LEU:HG	2.47	0.49
1:A:359:GLU:HG3	1:A:361:GLY:H	1.78	0.49
1:B:172:TRP:O	1:B:176:LEU:CD2	2.61	0.48
1:A:159:ALA:HB2	1:A:167:PHE:CE1	2.49	0.48
1:A:36:GLU:CD	1:A:36:GLU:H	2.17	0.48
1:A:70:GLY:HA2	1:A:360:LEU:O	2.14	0.48
1:B:95:GLY:HA3	1:B:98:MET:HE3	1.95	0.48
1:A:173:ASN:N	1:A:173:ASN:HD22	2.05	0.48
1:A:93:ARG:HG3	1:A:99:PHE:CE1	2.48	0.48
1:B:55:PHE:H	1:B:371:LEU:HG	1.79	0.48
1:B:55:PHE:N	1:B:371:LEU:HG	2.29	0.48
1:A:327:ARG:NH2	1:A:328:SER:OG	2.46	0.47
1:B:278:ASN:H	1:B:278:ASN:ND2	2.12	0.47
1:A:300:ILE:HG22	1:A:304:LYS:HE3	1.97	0.47
1:A:173:ASN:ND2	1:A:173:ASN:N	2.62	0.47
1:B:43:ARG:NH1	1:B:43:ARG:HG2	2.29	0.47
1:B:218:MET:CE	1:B:218:MET:HA	2.45	0.47
1:A:246:GLN:HE21	1:A:246:GLN:HB2	1.54	0.46
1:A:95:GLY:HA3	1:A:98:MET:CE	2.46	0.46
1:B:54:HIS:H	1:B:371:LEU:HD21	1.80	0.46
1:B:42:HIS:HA	1:B:366:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLU:HG3	1:B:39:VAL:O	2.15	0.46
1:A:210:THR:HB	1:A:213:THR:CG2	2.45	0.46
1:A:26:ARG:NH2	1:A:41:GLU:OE1	2.48	0.46
1:B:22:PRO:HA	1:B:369:ASP:OD2	2.15	0.46
1:A:192:GLU:HA	1:A:192:GLU:OE2	2.16	0.46
1:B:176:LEU:N	1:B:176:LEU:CD2	2.79	0.46
1:A:213:THR:HG23	1:A:215:GLN:H	1.81	0.46
1:A:178:GLN:C	1:A:180:ARG:HG2	2.35	0.46
1:B:342:GLN:O	1:B:346:GLU:HG3	2.16	0.46
1:A:175:LEU:HD23	1:A:175:LEU:O	2.16	0.45
1:A:327:ARG:HG2	1:A:328:SER:N	2.32	0.45
1:B:118:HIS:CG	1:B:118:HIS:O	2.68	0.45
1:B:320:PHE:HB3	1:B:334:PHE:CE1	2.52	0.45
1:A:142:LEU:CD2	1:A:186:MET:HG2	2.46	0.45
1:A:247:PRO:HB3	1:A:284:TYR:CD1	2.51	0.45
1:B:186:MET:CE	1:B:190:LEU:HD12	2.47	0.45
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.31	0.45
1:A:83:GLN:HB2	1:A:83:GLN:HE21	1.64	0.44
1:B:238:THR:OG1	1:B:275:LEU:HD12	2.17	0.44
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.81	0.44
1:A:60:LEU:HD13	1:A:83:GLN:HB2	1.99	0.44
2:B:372:SO4:O1	1:A:222:LYS:CE	2.65	0.44
1:B:138:PHE:O	1:B:142:LEU:HG	2.17	0.44
1:B:247:PRO:HB3	1:B:284:TYR:CG	2.52	0.44
1:B:95:GLY:HA3	1:B:98:MET:HE2	1.98	0.44
1:A:93:ARG:HD2	1:A:137:ASP:OD1	2.18	0.44
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.83	0.44
1:A:213:THR:HG23	1:A:215:GLN:HB2	1.99	0.44
1:A:173:ASN:HD22	1:A:174:GLN:N	2.16	0.43
1:A:325:LYS:HG3	1:A:327:ARG:NH2	2.28	0.43
1:B:312:TRP:CE3	1:B:319:HIS:CE1	3.06	0.43
1:B:371:LEU:HA	1:B:371:LEU:HD22	1.80	0.43
1:B:202:LEU:HD12	1:B:202:LEU:N	2.34	0.43
1:A:99:PHE:CZ	1:A:147:GLU:HG2	2.54	0.43
1:A:213:THR:HG23	1:A:215:GLN:N	2.34	0.43
1:A:137:ASP:O	1:A:141:VAL:HG23	2.19	0.42
1:B:86:PRO:HD2	1:B:126:PRO:HA	2.00	0.42
1:B:186:MET:HE1	1:B:190:LEU:HD12	2.01	0.42
1:B:370:LEU:O	1:B:371:LEU:CB	2.51	0.42
1:A:180:ARG:N	1:A:180:ARG:CD	2.82	0.42
1:B:253:LEU:HD22	1:B:343:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:O	1:A:215:GLN:HG3	2.20	0.42
1:B:221:HIS:O	1:B:225:GLU:HG3	2.20	0.42
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.35	0.42
2:B:372:SO4:O1	1:A:222:LYS:HE2	2.20	0.41
1:A:241:TYR:CB	1:A:250:ASN:O	2.66	0.41
1:B:282:MET:HE3	1:B:292:GLU:O	2.20	0.41
1:B:78:GLY:O	1:B:122:LEU:HD12	2.20	0.41
1:B:197:ALA:O	1:B:198:ARG:HB2	2.18	0.41
1:A:286:THR:CG2	1:A:286:THR:O	2.61	0.41
1:B:107:VAL:HG23	1:B:112:MET:CE	2.50	0.41
1:B:239:TYR:HA	1:B:251:ALA:HB2	2.02	0.41
1:A:195:HIS:HE1	1:A:230:VAL:O	2.04	0.41
1:B:246:GLN:HE21	1:B:246:GLN:HB2	1.58	0.41
1:B:21:LYS:O	1:B:26:ARG:HD2	2.21	0.41
1:A:131:GLU:O	1:A:132:ASP:HB2	2.21	0.41
1:A:359:GLU:HG2	1:A:362:GLN:OE1	2.20	0.41
1:B:282:MET:HE2	1:B:291:ARG:CD	2.47	0.40
1:B:144:SER:HB3	1:B:147:GLU:HG3	2.02	0.40
1:A:140:ASN:HD22	1:A:140:ASN:N	2.19	0.40
1:A:359:GLU:HG2	1:A:362:GLN:HG3	2.03	0.40
1:A:42:HIS:CE1	1:A:43:ARG:HG3	2.56	0.40
1:B:282:MET:HB3	1:B:282:MET:HE2	1.87	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	356/393 (91%)	338 (95%)	16 (4%)	2 (1%)	25	50
1	B	356/393 (91%)	336 (94%)	19 (5%)	1 (0%)	41	66
All	All	712/786 (91%)	674 (95%)	35 (5%)	3 (0%)	34	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	A	68	SER
1	B	286	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	316/344 (92%)	286 (90%)	30 (10%)	8	20
1	B	316/344 (92%)	288 (91%)	28 (9%)	9	22
All	All	632/688 (92%)	574 (91%)	58 (9%)	9	21

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	THR
1	B	33	LEU
1	B	39	VAL
1	B	59	VAL
1	B	93	ARG
1	B	113	ARG
1	B	129	LEU
1	B	160	LYS
1	B	169	VAL
1	B	180	ARG
1	B	186	MET
1	B	190	LEU
1	B	196	GLN
1	B	198	ARG
1	B	213	THR
1	B	215	GLN
1	B	218	MET
1	B	236	LEU
1	B	246	GLN
1	B	289	ASP

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Mol	Chain	Res	Type
1	B	292	GLU
1	B	294	VAL
1	B	308	PRO
1	B	325	LYS
1	B	359	GLU
1	B	360	LEU
1	B	366	TYR
1	B	371	LEU
1	A	12	LEU
1	A	17	GLN
1	A	24	GLN
1	A	29	VAL
1	A	33	LEU
1	A	39	VAL
1	A	59	VAL
1	A	83	GLN
1	A	96	ARG
1	A	107	VAL
1	A	113	ARG
1	A	145	GLU
1	A	146	ASP
1	A	173	ASN
1	A	175	LEU
1	A	186	MET
1	A	190	LEU
1	A	194	LEU
1	A	213	THR
1	A	236	LEU
1	A	246	GLN
1	A	289	ASP
1	A	294	VAL
1	A	307	ARG
1	A	325	LYS
1	A	327	ARG
1	A	350	GLU
1	A	355	VAL
1	A	359	GLU
1	A	366	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	HIS
1	B	54	HIS
1	B	157	GLN
1	B	246	GLN
1	B	278	ASN
1	B	301	GLN
1	A	24	GLN
1	A	42	HIS
1	A	54	HIS
1	A	83	GLN
1	A	109	GLN
1	A	173	ASN
1	A	178	GLN
1	A	189	HIS
1	A	215	GLN
1	A	246	GLN

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	B	373	-	4,4,4	0.49	0	6,6,6	0.77	0
2	SO4	B	372	-	4,4,4	0.44	0	6,6,6	0.60	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	372	SO4	2	0

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	360/393 (91%)	0.09	12 (3%)	46	46	26, 41, 69, 86	0
1	B	360/393 (91%)	-0.02	9 (2%)	57	59	27, 42, 66, 89	0
All	All	720/786 (91%)	0.04	21 (2%)	51	52	26, 42, 68, 89	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	LEU	5.1
1	A	177	SER	4.9
1	B	179	LYS	4.4
1	B	328	SER	3.9
1	B	176	LEU	3.6
1	A	178	GLN	3.4
1	A	175	LEU	3.2
1	A	174	GLN	3.1
1	A	135	TYR	2.9
1	A	139	ARG	2.9
1	A	288	LYS	2.7
1	B	118	HIS	2.7
1	A	245	HIS	2.6
1	B	119	ALA	2.5
1	A	96	ARG	2.5
1	B	326	SER	2.4
1	B	324	LYS	2.3
1	A	140	ASN	2.3
1	B	245	HIS	2.3
1	A	180	ARG	2.1
1	B	327	ARG	2.0

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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. 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	B-factors(Å^2)	Q<0.9
2	SO4	B	373	5/5	0.97	0.29	20,20,20,20	0
2	SO4	B	372	5/5	0.98	0.19	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.