Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 04:02 PM EDT

PDB ID	:	8SDP
Title	:	HTRA-1 PDSA bound to CKP 3A7
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Deposited on	:	2023-04-07
Resolution	:	2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

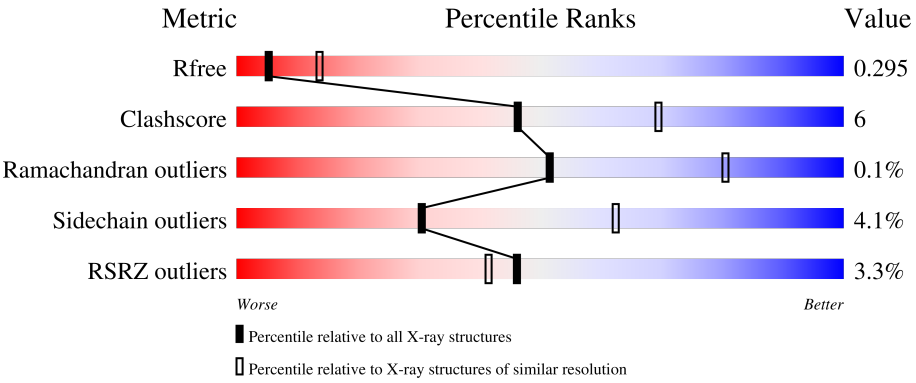
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.87 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	240	3% 70% 15% 15%
1	B	240	3% 67% 13% 20%
1	C	240	% 68% 11% 20%
2	I	37	73% 14% 14%
2	X	37	3% 68% 22% 11%

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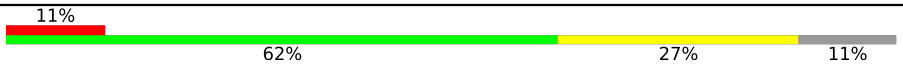
Mol	Chain	Length	Quality of chain
2	Y	37	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4826 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 Serine protease HTRA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1446	911	248	286	1			
1	B	193	Total	C	N	O		0	0	0
			1389	882	236	271				
1	C	191	Total	C	N	O		0	0	0
			1279	804	219	256				

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	expression tag	UNP Q92743
A	141	GLY	-	expression tag	UNP Q92743
A	142	SER	-	expression tag	UNP Q92743
A	143	SER	-	expression tag	UNP Q92743
A	144	HIS	-	expression tag	UNP Q92743
A	145	HIS	-	expression tag	UNP Q92743
A	146	HIS	-	expression tag	UNP Q92743
A	147	HIS	-	expression tag	UNP Q92743
A	148	HIS	-	expression tag	UNP Q92743
A	149	HIS	-	expression tag	UNP Q92743
A	150	SER	-	expression tag	UNP Q92743
A	151	SER	-	expression tag	UNP Q92743
A	152	GLY	-	expression tag	UNP Q92743
A	153	LEU	-	expression tag	UNP Q92743
A	154	VAL	-	expression tag	UNP Q92743
A	155	PRO	-	expression tag	UNP Q92743
A	156	ARG	-	expression tag	UNP Q92743
A	157	GLY	-	expression tag	UNP Q92743
A	158	SER	-	expression tag	UNP Q92743
A	159	HIS	-	expression tag	UNP Q92743
A	160	MET	-	expression tag	UNP Q92743
A	328	ALA	SER	engineered mutation	UNP Q92743
B	140	MET	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	expression tag	UNP Q92743
B	142	SER	-	expression tag	UNP Q92743
B	143	SER	-	expression tag	UNP Q92743
B	144	HIS	-	expression tag	UNP Q92743
B	145	HIS	-	expression tag	UNP Q92743
B	146	HIS	-	expression tag	UNP Q92743
B	147	HIS	-	expression tag	UNP Q92743
B	148	HIS	-	expression tag	UNP Q92743
B	149	HIS	-	expression tag	UNP Q92743
B	150	SER	-	expression tag	UNP Q92743
B	151	SER	-	expression tag	UNP Q92743
B	152	GLY	-	expression tag	UNP Q92743
B	153	LEU	-	expression tag	UNP Q92743
B	154	VAL	-	expression tag	UNP Q92743
B	155	PRO	-	expression tag	UNP Q92743
B	156	ARG	-	expression tag	UNP Q92743
B	157	GLY	-	expression tag	UNP Q92743
B	158	SER	-	expression tag	UNP Q92743
B	159	HIS	-	expression tag	UNP Q92743
B	160	MET	-	expression tag	UNP Q92743
B	328	ALA	SER	engineered mutation	UNP Q92743
C	140	MET	-	expression tag	UNP Q92743
C	141	GLY	-	expression tag	UNP Q92743
C	142	SER	-	expression tag	UNP Q92743
C	143	SER	-	expression tag	UNP Q92743
C	144	HIS	-	expression tag	UNP Q92743
C	145	HIS	-	expression tag	UNP Q92743
C	146	HIS	-	expression tag	UNP Q92743
C	147	HIS	-	expression tag	UNP Q92743
C	148	HIS	-	expression tag	UNP Q92743
C	149	HIS	-	expression tag	UNP Q92743
C	150	SER	-	expression tag	UNP Q92743
C	151	SER	-	expression tag	UNP Q92743
C	152	GLY	-	expression tag	UNP Q92743
C	153	LEU	-	expression tag	UNP Q92743
C	154	VAL	-	expression tag	UNP Q92743
C	155	PRO	-	expression tag	UNP Q92743
C	156	ARG	-	expression tag	UNP Q92743
C	157	GLY	-	expression tag	UNP Q92743
C	158	SER	-	expression tag	UNP Q92743
C	159	HIS	-	expression tag	UNP Q92743
C	160	MET	-	expression tag	UNP Q92743

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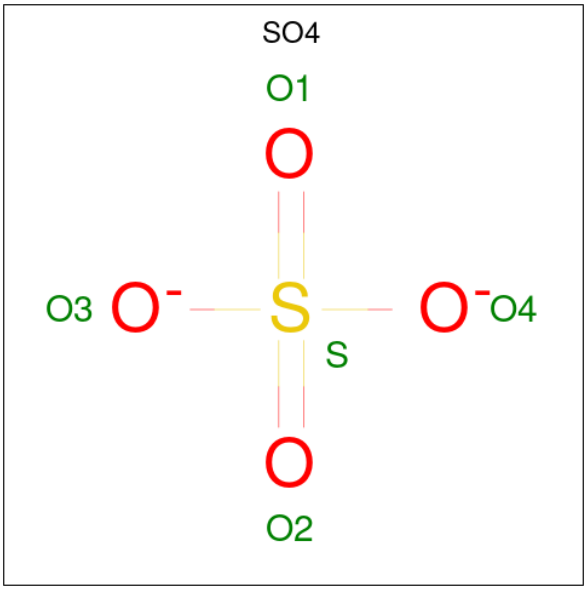
Chain	Residue	Modelled	Actual	Comment	Reference
C	328	ALA	SER	engineered mutation	UNP Q92743

- Molecule 2 is a protein called Cysteine knot peptide 3A7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	32	Total	C	N	O	S	0	0	0
			233	147	42	38	6			
2	X	33	Total	C	N	O	S	0	0	0
			234	144	40	44	6			
2	Y	33	Total	C	N	O	S	0	0	0
			240	153	39	42	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

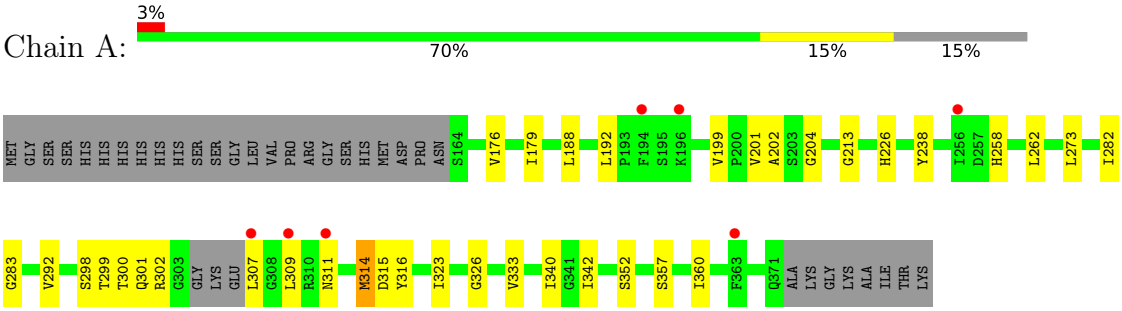


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	O	S		0	0
			5	4	1			

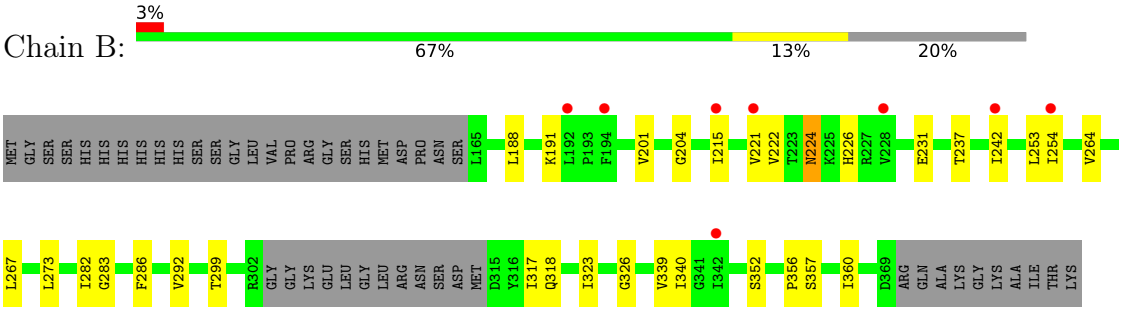
3 Residue-property plots (i)

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.

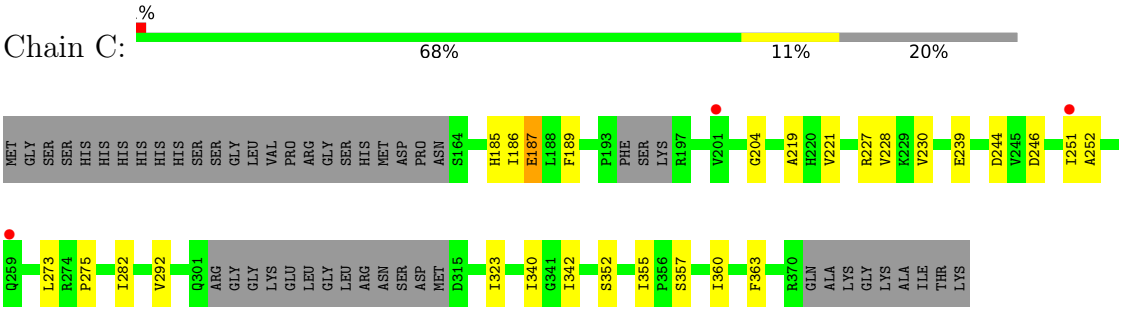
• Molecule 1: Serine protease HTRA1



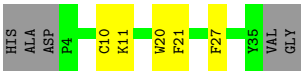
• Molecule 1: Serine protease HTRA1



• Molecule 1: Serine protease HTRA1

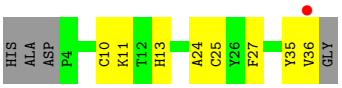


• Molecule 2: Cysteine knot peptide 3A7



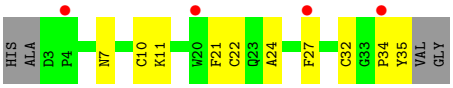
• Molecule 2: Cysteine knot peptide 3A7

Chain X:



• Molecule 2: Cysteine knot peptide 3A7

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.27Å 86.79Å 199.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.92 – 2.87 46.92 – 2.87	Depositor EDS
% Data completeness (in resolution range)	57.5 (46.92-2.87) 57.5 (46.92-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.87 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.276 , 0.295 0.276 , 0.295	Depositor DCC
R_{free} test set	562 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	87.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4826	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.28	0/1467	0.50	0/2006
1	B	0.25	0/1412	0.49	0/1936
1	C	0.24	0/1297	0.47	0/1783
2	I	0.27	0/243	0.51	0/332
2	X	0.27	0/242	0.51	0/331
2	Y	0.29	0/251	0.52	0/346
All	All	0.26	0/4912	0.49	0/6734

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

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	1446	0	1353	17	0
1	B	1389	0	1317	18	0
1	C	1279	0	1119	17	0
2	I	233	0	181	2	0
2	X	234	0	182	6	0
2	Y	240	0	176	5	0
3	B	5	0	0	0	0
All	All	4826	0	4328	58	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 6.

All (58) 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:C:185:HIS:CE1	1:C:187:GLU:HG3	2.25	0.71
1:C:282:ILE:HG13	1:C:292:VAL:HG22	1.73	0.68
1:A:357:SER:HA	1:A:360:ILE:HD12	1.81	0.62
1:A:176:VAL:HG11	1:C:275:PRO:HB2	1.82	0.62
2:X:24:ALA:HB2	2:X:36:VAL:HG22	1.84	0.60
1:C:185:HIS:HE1	1:C:187:GLU:HG3	1.67	0.59
1:C:323:ILE:HD12	1:C:352:SER:HB3	1.88	0.56
1:A:282:ILE:HG13	1:A:292:VAL:HG22	1.87	0.55
2:Y:10:CYS:SG	2:Y:11:LYS:N	2.80	0.55
1:B:201:VAL:HG21	1:B:226:HIS:ND1	2.22	0.55
1:A:273:LEU:HD21	1:A:340:ILE:HG21	1.89	0.55
1:C:357:SER:HA	1:C:360:ILE:HD12	1.89	0.54
1:B:282:ILE:HG13	1:B:292:VAL:HG22	1.89	0.54
1:B:317:ILE:HG12	1:B:356:PRO:HG3	1.90	0.54
1:B:357:SER:HA	1:B:360:ILE:HD12	1.90	0.53
1:B:222:VAL:HG12	1:B:242:ILE:HD13	1.91	0.52
2:X:10:CYS:SG	2:X:11:LYS:N	2.83	0.52
2:I:10:CYS:SG	2:I:11:LYS:N	2.84	0.51
1:B:323:ILE:HD12	1:B:352:SER:HB3	1.93	0.51
1:B:231:GLU:HG2	1:B:237:THR:HG22	1.92	0.50
1:B:273:LEU:HD21	1:B:340:ILE:HG21	1.93	0.50
1:B:267:LEU:HD22	1:B:357:SER:HB2	1.92	0.50
1:B:215:ILE:HB	1:B:254:ILE:HG13	1.94	0.50
1:C:228:VAL:O	1:C:239:GLU:HG3	2.12	0.50
1:A:314:MET:HG2	2:X:35:TYR:CE1	2.47	0.50
1:A:314:MET:O	1:A:316:TYR:N	2.45	0.49
1:A:342:ILE:HG13	1:A:360:ILE:HD11	1.95	0.48
1:C:251:ILE:HD11	1:C:355:ILE:HG21	1.95	0.48
1:A:283:GLY:HA3	1:A:326:GLY:O	2.13	0.48
2:X:13:HIS:CE1	2:X:25:CYS:H	2.32	0.48
2:Y:22:CYS:HA	2:Y:34:PRO:HA	1.96	0.47
1:C:273:LEU:HD21	1:C:340:ILE:HG21	1.96	0.47
1:A:188:LEU:HB2	1:A:202:ALA:HB3	1.97	0.47
1:C:189:PHE:N	1:C:227:ARG:O	2.46	0.47
1:C:219:ALA:HA	1:C:252:ALA:HB2	1.97	0.47
1:B:224:ASN:HB3	1:B:226:HIS:CE1	2.50	0.47
1:B:286:PHE:HD1	2:X:36:VAL:HG12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ASP:HB2	1:C:363:PHE:CE1	2.51	0.46
1:B:188:LEU:HD11	1:B:221:VAL:HG23	1.98	0.46
1:C:221:VAL:HG12	2:Y:27:PHE:CE1	2.51	0.45
1:A:238:TYR:OH	1:A:258:HIS:ND1	2.45	0.45
1:C:342:ILE:HG13	1:C:360:ILE:HD11	1.99	0.45
1:B:204:GLY:HA3	2:X:27:PHE:CZ	2.52	0.44
1:A:323:ILE:HD12	1:A:352:SER:HB3	2.00	0.44
1:A:314:MET:H	1:A:314:MET:HG3	1.45	0.44
1:A:201:VAL:HG21	1:A:226:HIS:ND1	2.34	0.43
1:C:204:GLY:HA3	2:Y:27:PHE:CZ	2.54	0.43
1:B:299:THR:HG22	1:B:318:GLN:HB2	2.02	0.42
1:B:191:LYS:HA	1:B:191:LYS:HD3	1.88	0.42
1:A:204:GLY:HA3	2:I:27:PHE:CZ	2.55	0.41
2:Y:24:ALA:O	2:Y:32:CYS:HA	2.21	0.41
1:A:192:LEU:HD11	1:A:199:VAL:HG13	2.03	0.41
1:A:179:ILE:HG21	1:A:333:VAL:HG11	2.03	0.41
1:A:213:GLY:HA2	1:A:262:LEU:HD13	2.03	0.41
1:C:186:ILE:HG12	1:C:230:VAL:HG22	2.03	0.40
1:B:267:LEU:HD23	1:B:339:VAL:HB	2.03	0.40
1:B:283:GLY:HA3	1:B:326:GLY:O	2.21	0.40
1:C:246:ASP:HB2	1:C:363:PHE:CD1	2.56	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	201/240 (84%)	191 (95%)	9 (4%)	1 (0%)	29 59
1	B	189/240 (79%)	187 (99%)	2 (1%)	0	100 100
1	C	185/240 (77%)	181 (98%)	4 (2%)	0	100 100
2	I	30/37 (81%)	26 (87%)	4 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	X	31/37 (84%)	28 (90%)	3 (10%)	0	100 100
2	Y	31/37 (84%)	28 (90%)	3 (10%)	0	100 100
All	All	667/831 (80%)	641 (96%)	25 (4%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ASN

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	143/202 (71%)	134 (94%)	9 (6%)	18 44
1	B	141/202 (70%)	138 (98%)	3 (2%)	53 80
1	C	113/202 (56%)	111 (98%)	2 (2%)	59 83
2	I	21/30 (70%)	19 (90%)	2 (10%)	8 24
2	X	23/30 (77%)	23 (100%)	0	100 100
2	Y	22/30 (73%)	19 (86%)	3 (14%)	3 10
All	All	463/696 (66%)	444 (96%)	19 (4%)	30 62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	SER
1	A	299	THR
1	A	300	THR
1	A	301	GLN
1	A	302	ARG
1	A	307	LEU
1	A	309	LEU
1	A	314	MET
1	A	315	ASP

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Mol	Chain	Res	Type
1	B	224	ASN
1	B	253	LEU
1	B	264	VAL
1	C	187	GLU
1	C	244	ASP
2	I	20	TRP
2	I	21	PHE
2	Y	7	ASN
2	Y	21	PHE
2	Y	35	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	185	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
3	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.04	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.

No monomer is involved in short contacts.

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	205/240 (85%)	0.21	7 (3%) 45 40	50, 69, 106, 158	0
1	B	193/240 (80%)	0.22	8 (4%) 37 32	56, 74, 97, 126	0
1	C	191/240 (79%)	0.28	3 (1%) 72 71	58, 80, 108, 125	0
2	I	32/37 (86%)	0.02	0 100 100	73, 87, 100, 108	0
2	X	33/37 (89%)	-0.08	1 (3%) 50 46	65, 75, 81, 89	0
2	Y	33/37 (89%)	0.40	4 (12%) 4 2	81, 98, 121, 127	0
All	All	687/831 (82%)	0.22	23 (3%) 46 41	50, 76, 108, 158	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259	GLN	4.9
1	B	242	ILE	3.4
1	A	309	LEU	3.2
1	A	307	LEU	3.2
1	B	254	ILE	3.0
1	C	201	VAL	2.9
1	B	342	ILE	2.9
1	A	196	LYS	2.8
2	Y	27	PHE	2.7
1	B	221	VAL	2.7
1	B	228	VAL	2.6
1	A	363	PHE	2.6
2	Y	34	PRO	2.4
1	A	311	ASN	2.4
1	C	251	ILE	2.3
1	B	194	PHE	2.3
1	B	192	LEU	2.2
2	Y	20	TRP	2.1
1	A	256	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	Y	4	PRO	2.1
1	A	194	PHE	2.1
2	X	36	VAL	2.0
1	B	215	ILE	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)

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, 95^{th} 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
3	SO4	B	401	5/5	0.96	0.10	91,91,91,91	0

6.5 Other polymers (i)

There are no such residues in this entry.