



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 03:31 PM EDT

PDB ID : 3UGX
Title : Crystal Structure of Visual Arrestin
Authors : Batra-Safferling, R.; Granzin, J.
Deposited on : unknown
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

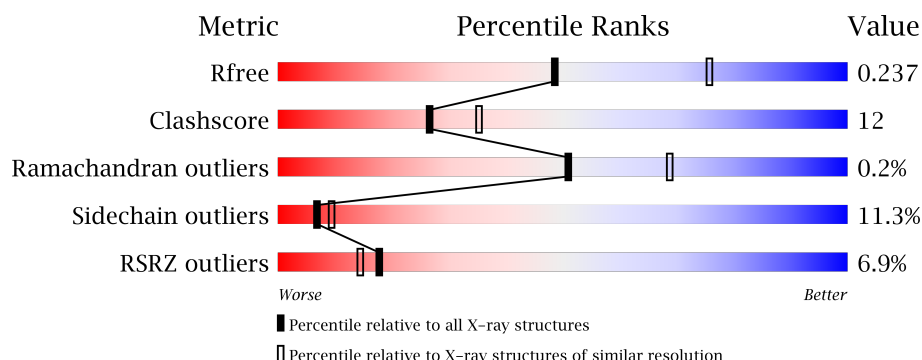
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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 $\leq 5\%$. 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	414	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	414	<div> <div>8%</div> <div> <div></div> <div>56%</div> <div>26%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	414	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	414	<div> <div>9%</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTD	A	406	-	-	-	X
2	PTD	A	408	-	-	-	X
2	PTD	A	410	-	-	X	X
2	PTD	A	411	-	-	-	X
2	PTD	C	405	-	-	-	X
2	PTD	C	406	-	-	X	X
2	PTD	C	407	-	-	-	X
4	EDO	B	409	-	-	-	X
4	EDO	C	409	-	-	-	X
4	EDO	C	411	-	-	-	X
4	EDO	D	408	-	-	-	X
5	IMD	B	405	-	-	X	X
5	IMD	D	405	-	-	-	X
5	IMD	D	406	-	-	-	X
6	K	C	408	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11230 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 S-arrestin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	1	0
			2859	1832	474	544	9			
1	B	352	Total	C	N	O	S	0	0	0
			2662	1709	437	507	9			
1	C	358	Total	C	N	O	S	0	0	0
			2772	1783	461	520	8			
1	D	348	Total	C	N	O	S	0	0	0
			2608	1680	432	487	9			

There are 40 discrepancies between the modelled and reference sequences:

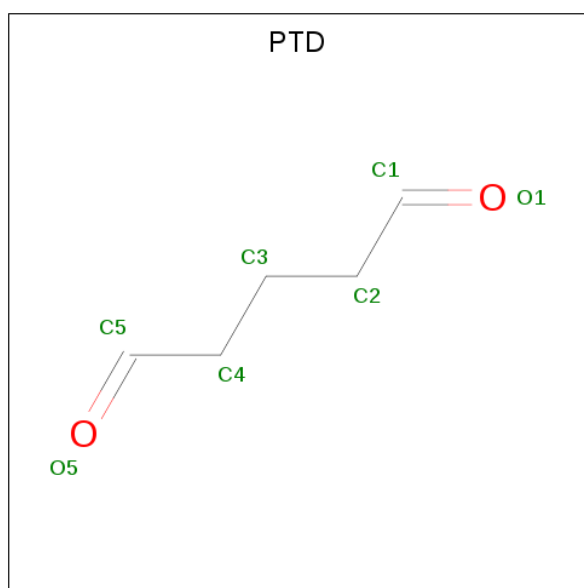
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	EXPRESSION TAG	UNP P08168
A	-8	SER	-	EXPRESSION TAG	UNP P08168
A	-7	TRP	-	EXPRESSION TAG	UNP P08168
A	-6	SER	-	EXPRESSION TAG	UNP P08168
A	-5	HIS	-	EXPRESSION TAG	UNP P08168
A	-4	PRO	-	EXPRESSION TAG	UNP P08168
A	-3	GLN	-	EXPRESSION TAG	UNP P08168
A	-2	PHE	-	EXPRESSION TAG	UNP P08168
A	-1	GLU	-	EXPRESSION TAG	UNP P08168
A	0	LYS	-	EXPRESSION TAG	UNP P08168
B	-9	ALA	-	EXPRESSION TAG	UNP P08168
B	-8	SER	-	EXPRESSION TAG	UNP P08168
B	-7	TRP	-	EXPRESSION TAG	UNP P08168
B	-6	SER	-	EXPRESSION TAG	UNP P08168
B	-5	HIS	-	EXPRESSION TAG	UNP P08168
B	-4	PRO	-	EXPRESSION TAG	UNP P08168
B	-3	GLN	-	EXPRESSION TAG	UNP P08168
B	-2	PHE	-	EXPRESSION TAG	UNP P08168
B	-1	GLU	-	EXPRESSION TAG	UNP P08168
B	0	LYS	-	EXPRESSION TAG	UNP P08168
C	-9	ALA	-	EXPRESSION TAG	UNP P08168

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	EXPRESSION TAG	UNP P08168
C	-7	TRP	-	EXPRESSION TAG	UNP P08168
C	-6	SER	-	EXPRESSION TAG	UNP P08168
C	-5	HIS	-	EXPRESSION TAG	UNP P08168
C	-4	PRO	-	EXPRESSION TAG	UNP P08168
C	-3	GLN	-	EXPRESSION TAG	UNP P08168
C	-2	PHE	-	EXPRESSION TAG	UNP P08168
C	-1	GLU	-	EXPRESSION TAG	UNP P08168
C	0	LYS	-	EXPRESSION TAG	UNP P08168
D	-9	ALA	-	EXPRESSION TAG	UNP P08168
D	-8	SER	-	EXPRESSION TAG	UNP P08168
D	-7	TRP	-	EXPRESSION TAG	UNP P08168
D	-6	SER	-	EXPRESSION TAG	UNP P08168
D	-5	HIS	-	EXPRESSION TAG	UNP P08168
D	-4	PRO	-	EXPRESSION TAG	UNP P08168
D	-3	GLN	-	EXPRESSION TAG	UNP P08168
D	-2	PHE	-	EXPRESSION TAG	UNP P08168
D	-1	GLU	-	EXPRESSION TAG	UNP P08168
D	0	LYS	-	EXPRESSION TAG	UNP P08168

- Molecule 2 is PENTANEDIAL (three-letter code: PTD) (formula: C₅H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	5	2		
2	A	1	Total	C	O	0	0
			7	5	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	A	1	Total C O 7 5 2	0	0
2	B	1	Total C O 7 5 2	0	0
2	B	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	C	1	Total C O 7 5 2	0	0
2	D	1	Total C O 7 5 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

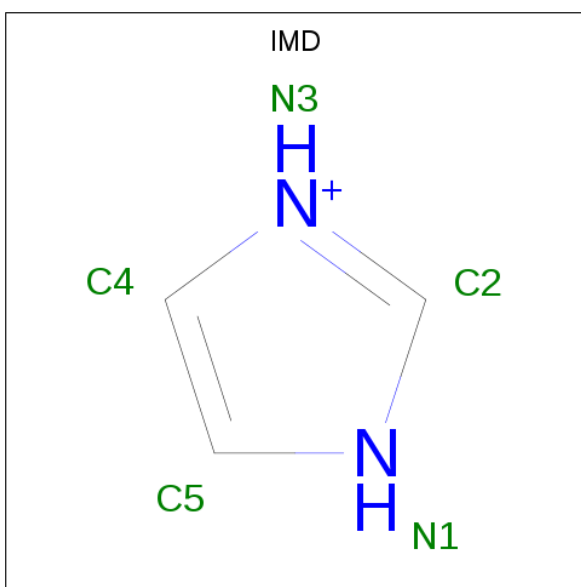
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	K	0	0
			1	1		

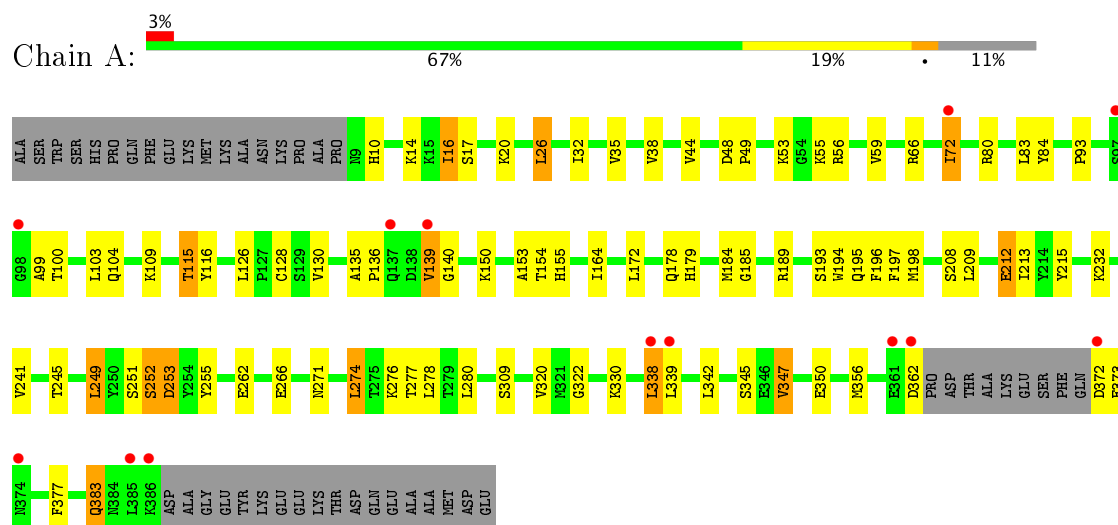
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total	O	0	0
			68	68		
7	B	31	Total	O	0	0
			31	31		
7	C	45	Total	O	0	0
			45	45		
7	D	41	Total	O	0	0
			41	41		

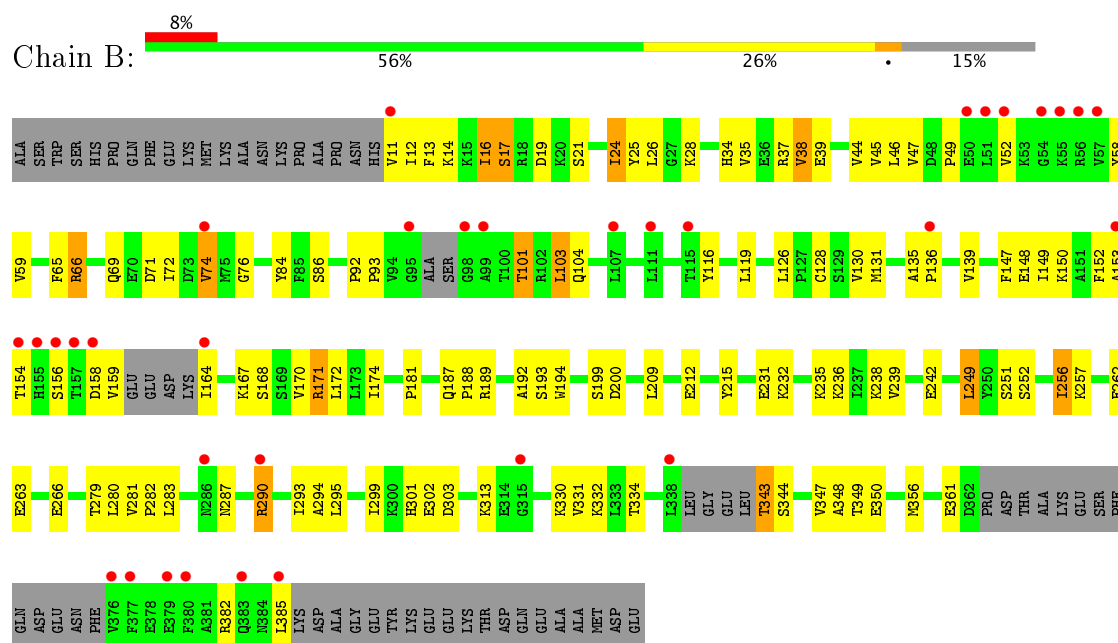
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

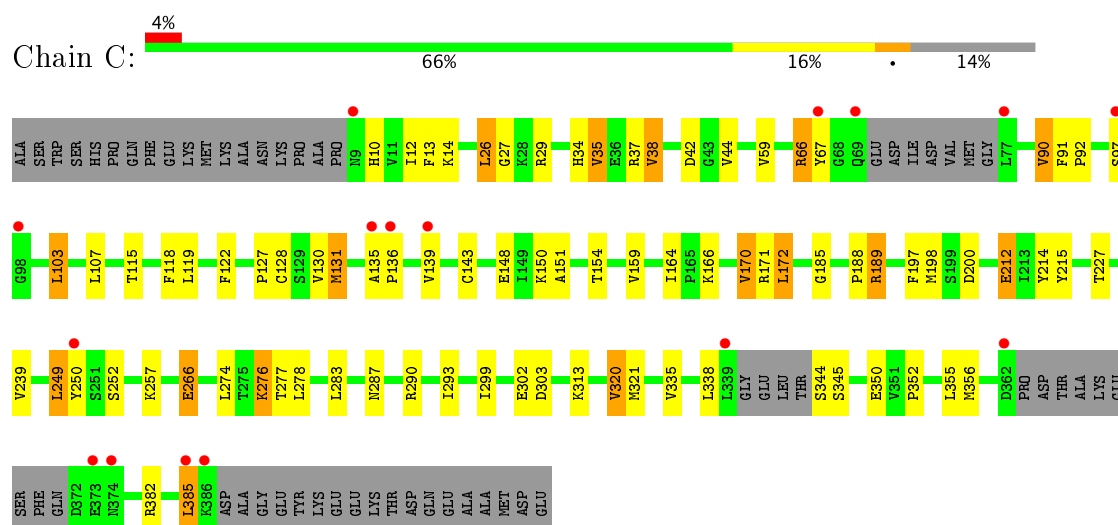
• Molecule 1: S-arrestin



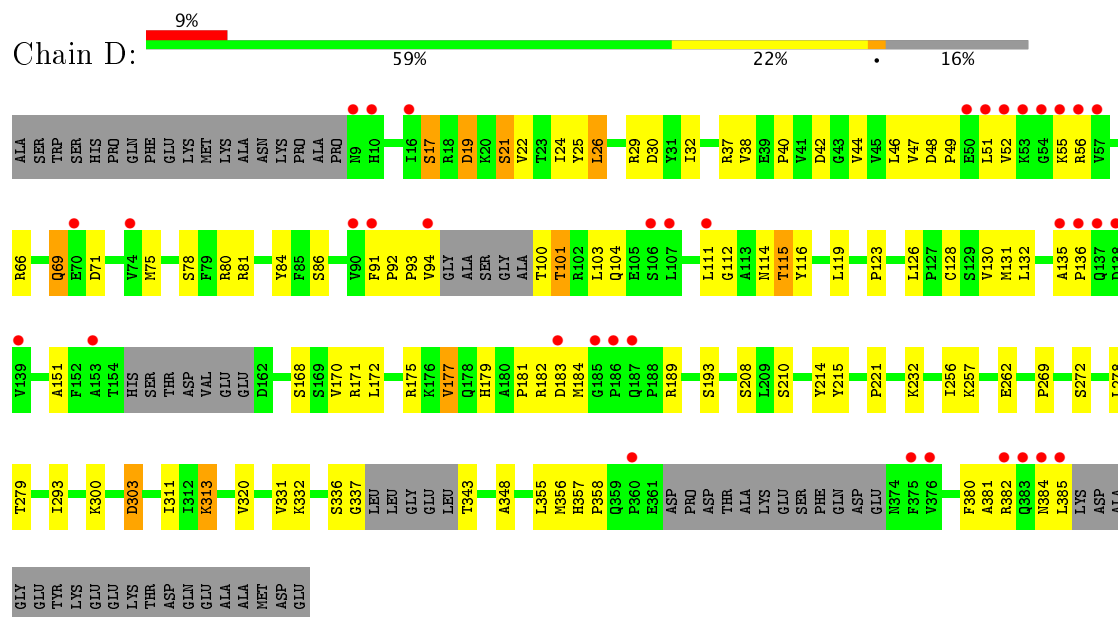
• Molecule 1: S-arrestin



• Molecule 1: S-arrestin



• Molecule 1: S-arrestin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.36Å 184.33Å 90.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.89 – 2.65 32.89 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (32.89-2.65) 98.3 (32.89-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.209 , 0.253 0.189 , 0.237	Depositor DCC
R_{free} test set	4062 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11230	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, K, PTD, IMD, EDO

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	0.42	0/2919	0.62	0/3969
1	B	0.38	0/2712	0.58	0/3698
1	C	0.40	0/2827	0.59	0/3841
1	D	0.42	0/2660	0.60	0/3632
All	All	0.40	0/11118	0.60	0/15140

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	2859	0	2852	57	0
1	B	2662	0	2615	77	0
1	C	2772	0	2776	55	0
1	D	2608	0	2538	68	0
2	A	56	0	64	13	0
2	B	14	0	16	0	0
2	C	21	0	24	11	0
2	D	7	0	8	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	8	0	12	1	0
4	B	4	0	6	0	0
4	C	12	0	18	1	0
4	D	4	0	6	2	0
5	B	5	0	5	4	0
5	D	10	0	10	4	0
6	C	1	0	0	0	0
7	A	68	0	0	1	0
7	B	31	0	0	2	0
7	C	45	0	0	4	0
7	D	41	0	0	1	0
All	All	11230	0	10950	255	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 12.

All (255) 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:D:128:CYS:H	5:D:406:IMD:H5	1.14	1.07
1:A:128:CYS:HB2	2:A:410:PTD:HC31	1.53	0.91
1:D:313:LYS:HG2	7:D:442:HOH:O	1.70	0.90
1:A:72:ILE:HG21	1:A:80:ARG:HD2	1.57	0.87
1:D:128:CYS:H	5:D:406:IMD:C5	1.88	0.86
1:C:352:PRO:HB2	2:C:407:PTD:HC5	1.59	0.85
1:C:154:THR:HG22	1:C:164:ILE:HG12	1.60	0.82
1:D:128:CYS:N	5:D:406:IMD:H5	1.94	0.81
1:B:84:TYR:HB2	1:B:126:LEU:HD21	1.66	0.78
1:B:93:PRO:HG3	1:B:116:TYR:CD2	2.20	0.77
1:D:311:ILE:HG22	1:D:313:LYS:HE2	1.68	0.76
1:B:290:ARG:NH1	1:B:299:ILE:O	2.21	0.73
1:A:55:LYS:HE2	2:A:405:PTD:HC31	1.68	0.73
1:D:100:THR:HG22	1:D:101:THR:N	2.03	0.73
1:D:189:ARG:NH1	1:D:208:SER:OG	2.22	0.72
1:C:290:ARG:NH1	1:C:299:ILE:O	2.22	0.71
1:D:25:TYR:HB2	1:D:44:VAL:HG22	1.71	0.71
1:A:93:PRO:HG3	1:A:116:TYR:CE1	2.26	0.71
1:C:303:ASP:OD2	1:C:382:ARG:NH1	2.23	0.71
1:A:128:CYS:H	2:A:410:PTD:HC1	1.56	0.70
1:B:158:ASP:N	1:B:159:VAL:HA	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ARG:HH21	1:D:80:ARG:HD2	1.54	0.70
1:B:330:LYS:HD2	1:B:350:GLU:HG3	1.74	0.70
1:A:249:LEU:HD22	1:A:322:GLY:HA2	1.73	0.69
1:A:154:THR:HG22	1:A:164:ILE:HG12	1.75	0.68
1:A:16:ILE:HD11	1:A:20:LYS:HD3	1.75	0.68
1:A:26:LEU:HD22	1:A:172:LEU:HD23	1.75	0.68
1:C:252:SER:HB2	2:C:405:PTD:HC22	1.75	0.68
1:D:66:ARG:HB2	5:D:405:IMD:H2	1.74	0.68
1:B:93:PRO:CG	1:B:116:TYR:CD2	2.78	0.67
1:D:269:PRO:O	1:D:272:SER:HB3	1.94	0.67
1:D:66:ARG:HH21	1:D:80:ARG:HH11	1.41	0.67
1:A:55:LYS:CE	2:A:405:PTD:HC31	2.26	0.66
1:D:215:TYR:CZ	4:D:408:EDO:H21	2.33	0.64
1:D:135:ALA:HB1	1:D:136:PRO:HD2	1.79	0.64
1:C:148:GLU:OE2	1:C:171:ARG:NE	2.24	0.63
1:A:99:ALA:HB1	1:A:104:GLN:HB2	1.81	0.63
1:D:40:PRO:HB2	1:D:119:LEU:HD11	1.81	0.63
1:C:42:ASP:HB3	1:C:119:LEU:HD12	1.81	0.63
1:B:47:VAL:HB	1:B:52:VAL:HG11	1.81	0.62
1:B:101:THR:HG23	1:B:104:GLN:OE1	1.99	0.62
1:B:290:ARG:HD3	1:B:299:ILE:HG23	1.82	0.62
2:C:407:PTD:HC1	7:C:412:HOH:O	1.99	0.61
1:A:377:PHE:CD2	2:A:409:PTD:HC5	2.36	0.61
1:C:66:ARG:HH12	1:C:131:MET:CE	2.14	0.61
1:C:215:TYR:HA	1:C:356:MET:O	2.01	0.61
1:B:238:LYS:HG3	1:B:263:GLU:HB3	1.82	0.60
1:B:153:ALA:HB3	1:B:168:SER:HB3	1.83	0.60
1:A:55:LYS:HG2	1:A:155:HIS:HB3	1.84	0.60
1:A:16:ILE:HD11	1:A:20:LYS:HA	1.84	0.59
1:D:256:ILE:O	1:D:257:LYS:HD3	2.01	0.59
1:A:185:GLY:N	1:A:212:GLU:HG2	2.17	0.59
1:D:66:ARG:NH2	1:D:80:ARG:HD2	2.17	0.59
1:B:66:ARG:HG3	5:B:405:IMD:H2	1.84	0.59
4:A:415:EDO:O2	1:B:200:ASP:OD1	2.21	0.58
1:A:252:SER:OG	2:A:407:PTD:HC5	2.04	0.58
1:D:21:SER:HB2	1:D:51:LEU:HB2	1.86	0.58
1:A:274:LEU:HD12	1:B:347:VAL:HG12	1.86	0.58
1:D:100:THR:CG2	1:D:101:THR:N	2.67	0.58
1:A:277:THR:HB	1:B:343:THR:HG21	1.87	0.57
1:B:16:ILE:HG12	1:B:17:SER:N	2.19	0.57
1:B:74:VAL:O	2:C:406:PTD:O1	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:CB	2:A:407:PTD:HC5	2.35	0.56
1:A:178:GLN:OE1	2:A:410:PTD:HC5	2.05	0.56
1:A:383:GLN:CD	1:A:383:GLN:H	2.06	0.56
1:D:135:ALA:HB1	1:D:136:PRO:CD	2.36	0.56
1:A:55:LYS:HE2	2:A:405:PTD:HC1	1.88	0.56
1:D:84:TYR:CD1	1:D:123:PRO:HG3	2.40	0.56
1:A:215:TYR:HA	1:A:356:MET:O	2.05	0.56
1:C:26:LEU:HD22	1:C:172:LEU:HD23	1.87	0.55
1:D:303:ASP:N	1:D:303:ASP:OD1	2.34	0.55
1:B:128:CYS:O	1:B:130:VAL:HG23	2.07	0.55
1:B:194:TRP:CD2	1:B:349:THR:HG21	2.42	0.55
1:B:158:ASP:HB3	1:B:159:VAL:C	2.27	0.55
1:D:232:LYS:HD3	1:D:337:GLY:HA3	1.89	0.55
1:A:338:LEU:O	1:A:342:LEU:N	2.40	0.54
1:D:91:PHE:HA	1:D:92:PRO:C	2.27	0.54
1:B:294:ALA:O	1:B:295:LEU:HD23	2.08	0.54
1:A:184:MET:HB3	1:A:213:ILE:HD12	1.89	0.54
1:C:135:ALA:HB1	1:C:136:PRO:HD2	1.89	0.54
1:A:194:TRP:CE2	1:A:347:VAL:HG23	2.42	0.54
1:B:93:PRO:CG	1:B:116:TYR:CE2	2.91	0.54
1:A:330:LYS:HG3	1:A:350:GLU:HG3	1.89	0.54
1:D:21:SER:HB2	1:D:51:LEU:CB	2.38	0.54
1:C:185:GLY:N	1:C:212:GLU:HG2	2.23	0.54
1:D:19:ASP:OD2	1:D:21:SER:HB3	2.08	0.53
1:D:215:TYR:HA	1:D:356:MET:O	2.08	0.53
1:C:189:ARG:O	2:C:406:PTD:HC31	2.09	0.53
1:B:49:PRO:HA	1:B:52:VAL:HG22	1.90	0.53
1:D:52:VAL:O	1:D:55:LYS:HB2	2.07	0.53
1:A:185:GLY:H	1:A:212:GLU:HG2	1.74	0.52
1:C:66:ARG:HH12	1:C:131:MET:HE1	1.73	0.52
1:D:29:ARG:HG2	1:D:380:PHE:CE2	2.44	0.52
1:A:252:SER:OG	2:A:407:PTD:HC1	2.10	0.52
1:B:19:ASP:OD1	1:B:21:SER:HB3	2.09	0.52
1:B:135:ALA:HB1	1:B:136:PRO:HD2	1.92	0.52
1:B:148:GLU:OE2	1:B:171:ARG:HG3	2.08	0.52
1:B:313:LYS:HD2	1:B:313:LYS:N	2.25	0.52
1:B:28:LYS:NZ	1:B:39:GLU:OE2	2.43	0.52
1:B:239:VAL:HG12	1:B:280:LEU:HD11	1.92	0.52
5:B:405:IMD:N1	7:B:435:HOH:O	2.28	0.51
1:B:215:TYR:HA	1:B:356:MET:O	2.11	0.51
1:D:215:TYR:CZ	1:D:358:PRO:HA	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:GLU:OE2	1:C:276:LYS:NZ	2.23	0.51
1:D:93:PRO:HG3	1:D:116:TYR:CD2	2.46	0.51
1:B:58:TYR:HB2	1:B:152:PHE:CZ	2.45	0.51
1:D:46:LEU:HD13	1:D:115:THR:HG23	1.92	0.51
1:B:242:GLU:OE1	1:B:330:LYS:HD3	2.12	0.50
1:B:93:PRO:HG2	1:B:116:TYR:CE2	2.46	0.50
1:B:12:ILE:HD11	1:B:103:LEU:HD21	1.94	0.50
1:C:283:LEU:O	1:C:287:ASN:ND2	2.44	0.50
1:C:302:GLU:HA	1:C:385:LEU:HD13	1.94	0.50
1:A:197:PHE:CE1	1:D:84:TYR:HA	2.46	0.50
1:C:90:VAL:HG23	1:C:118:PHE:HB3	1.94	0.50
1:B:101:THR:N	1:B:104:GLN:OE1	2.41	0.50
1:D:300:LYS:O	1:D:384:ASN:HA	2.11	0.50
1:B:302:GLU:HA	1:B:385:LEU:HD13	1.94	0.50
1:B:238:LYS:HG3	1:B:263:GLU:CB	2.42	0.50
1:B:313:LYS:NZ	7:B:436:HOH:O	2.36	0.50
1:D:24:ILE:HD12	1:D:151:ALA:HB2	1.92	0.50
1:D:48:ASP:CG	1:D:51:LEU:HG	2.31	0.50
1:A:266:GLU:OE2	1:A:276:LYS:HE2	2.12	0.49
1:B:199:SER:O	1:B:200:ASP:HB2	2.12	0.49
1:C:320:VAL:HG13	7:C:443:HOH:O	2.12	0.49
1:C:128:CYS:O	1:C:130:VAL:HG23	2.11	0.49
1:D:331:VAL:O	1:D:348:ALA:HA	2.12	0.49
1:B:158:ASP:N	1:B:159:VAL:CA	2.75	0.49
1:D:32:ILE:HG12	1:D:179:HIS:CD2	2.47	0.49
1:A:128:CYS:O	1:A:130:VAL:HG23	2.13	0.49
1:C:335:VAL:O	1:C:344:SER:HA	2.12	0.49
1:C:166:LYS:HA	4:C:409:EDO:H11	1.94	0.49
1:A:241:VAL:HG23	1:A:280:LEU:HD13	1.94	0.48
1:D:91:PHE:HA	1:D:93:PRO:HD3	1.95	0.48
1:A:271:ASN:O	7:A:453:HOH:O	2.20	0.48
1:C:214:TYR:O	1:C:355:LEU:HD12	2.13	0.48
1:C:27:GLY:HA3	1:C:103:LEU:HD11	1.95	0.48
1:A:195:GLN:HB3	1:D:81:ARG:HG3	1.95	0.48
1:B:17:SER:OG	1:B:167:LYS:O	2.28	0.48
1:B:25:TYR:HB2	1:B:44:VAL:HG22	1.96	0.48
1:C:185:GLY:CA	1:C:212:GLU:HG2	2.44	0.48
1:B:189:ARG:HB3	1:B:209:LEU:O	2.15	0.47
1:B:331:VAL:O	1:B:348:ALA:HA	2.14	0.47
1:C:185:GLY:H	1:C:212:GLU:HG2	1.79	0.47
1:C:44:VAL:HB	1:C:115:THR:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:O	7:C:427:HOH:O	2.20	0.47
1:D:93:PRO:HG3	1:D:116:TYR:HD2	1.80	0.47
1:D:17:SER:OG	1:D:22:VAL:O	2.33	0.47
1:D:311:ILE:O	1:D:313:LYS:CE	2.63	0.46
1:A:56:ARG:O	1:A:153:ALA:HA	2.16	0.46
1:B:242:GLU:OE1	1:B:256:ILE:HD11	2.16	0.46
1:A:139:VAL:HG12	1:A:140:GLY:H	1.79	0.46
1:C:290:ARG:HD3	1:C:299:ILE:HG23	1.97	0.46
1:C:151:ALA:HB3	1:C:170:VAL:HG23	1.97	0.46
1:A:309:SER:O	2:A:410:PTD:HC42	2.15	0.46
1:D:100:THR:CG2	1:D:101:THR:H	2.29	0.46
1:A:197:PHE:CD2	1:A:198:MET:HG3	2.51	0.45
1:C:385:LEU:HA	1:C:385:LEU:HD12	1.80	0.45
1:C:274:LEU:HD23	1:C:274:LEU:C	2.36	0.45
1:A:185:GLY:CA	1:A:212:GLU:HG2	2.46	0.45
1:C:148:GLU:OE1	7:C:413:HOH:O	2.21	0.45
1:B:93:PRO:HG3	1:B:116:TYR:HD2	1.73	0.45
1:D:112:GLY:O	1:D:115:THR:OG1	2.32	0.45
1:B:34:HIS:O	1:B:181:PRO:HB3	2.16	0.45
1:C:188:PRO:HA	2:C:406:PTD:HC1	1.99	0.45
1:A:26:LEU:HD22	1:A:172:LEU:CD2	2.43	0.45
1:B:135:ALA:HB1	1:B:136:PRO:CD	2.46	0.45
1:D:215:TYR:CE2	4:D:408:EDO:H21	2.51	0.45
1:D:49:PRO:HG3	1:D:114:ASN:OD1	2.17	0.45
1:A:196:PHE:CE1	1:A:338:LEU:HD11	2.52	0.45
1:B:147:PHE:HB2	1:B:174:ILE:O	2.16	0.45
1:B:235:LYS:HA	1:B:266:GLU:O	2.17	0.45
1:D:311:ILE:O	1:D:313:LYS:HE3	2.16	0.45
1:D:215:TYR:CE1	1:D:358:PRO:HA	2.52	0.45
1:B:192:ALA:HB3	1:B:194:TRP:CH2	2.51	0.45
1:B:66:ARG:HG3	5:B:405:IMD:C2	2.47	0.45
1:C:34:HIS:O	1:C:35:VAL:HB	2.16	0.45
1:B:59:VAL:HA	1:B:150:LYS:O	2.17	0.45
1:C:276:LYS:HG3	1:C:277:THR:N	2.30	0.45
1:B:238:LYS:HE3	1:B:238:LYS:HB2	1.74	0.44
1:C:13:PHE:CE1	1:C:29:ARG:CZ	3.00	0.44
1:D:84:TYR:HB2	1:D:126:LEU:HD21	1.99	0.44
1:D:26:LEU:HA	1:D:26:LEU:HD12	1.82	0.44
1:D:30:ASP:OD1	1:D:175:ARG:HB2	2.18	0.44
1:D:278:LEU:HD12	1:D:278:LEU:C	2.38	0.44
1:D:42:ASP:HB3	1:D:119:LEU:HD13	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:CG2	2:A:410:PTD:HC21	2.47	0.44
1:B:25:TYR:HB2	1:B:44:VAL:CG2	2.47	0.44
1:A:44:VAL:HB	1:A:115:THR:HG22	2.00	0.44
1:C:91:PHE:HA	1:C:92:PRO:C	2.37	0.44
1:C:38:VAL:HG22	1:C:122:PHE:HB2	2.00	0.44
1:B:93:PRO:HG2	1:B:116:TYR:CD2	2.53	0.43
1:B:66:ARG:HB3	1:B:66:ARG:HE	1.30	0.43
1:B:92:PRO:HA	1:B:93:PRO:HD3	1.69	0.43
1:B:282:PRO:O	1:B:283:LEU:HG	2.18	0.43
1:B:187:GLN:HA	1:B:188:PRO:HD2	1.88	0.43
1:C:35:VAL:HG13	1:C:313:LYS:HE3	2.01	0.43
1:D:100:THR:HG22	1:D:101:THR:H	1.78	0.43
1:D:181:PRO:HG2	1:D:184:MET:HG3	2.00	0.43
1:B:37:ARG:HG2	1:B:38:VAL:N	2.32	0.43
1:D:48:ASP:O	1:D:52:VAL:HG22	2.18	0.43
1:B:13:PHE:O	1:B:25:TYR:HA	2.19	0.43
1:B:294:ALA:C	1:B:295:LEU:HD23	2.40	0.42
1:D:221:PRO:HA	1:D:278:LEU:O	2.19	0.42
1:D:29:ARG:HB3	1:D:382:ARG:NH2	2.34	0.42
1:D:66:ARG:NH1	1:D:69:GLN:OE1	2.52	0.42
1:C:249:LEU:HD12	1:C:249:LEU:HA	1.92	0.42
1:C:257:LYS:HG3	1:C:293:ILE:HG22	2.01	0.42
1:C:352:PRO:HD2	2:C:406:PTD:HC32	2.01	0.42
1:B:194:TRP:CZ2	1:B:349:THR:HB	2.54	0.42
1:C:135:ALA:HB1	1:C:136:PRO:CD	2.49	0.42
1:D:182:ARG:O	1:D:183:ASP:HB2	2.19	0.42
1:B:149:ILE:HD13	1:B:149:ILE:HA	1.91	0.42
1:B:301:HIS:CE1	1:B:382:ARG:HG3	2.54	0.42
1:A:84:TYR:HB2	1:A:126:LEU:HD21	2.01	0.42
1:D:19:ASP:CG	1:D:21:SER:HB3	2.41	0.42
1:A:14:LYS:NZ	2:A:409:PTD:HC41	2.35	0.42
1:A:262:GLU:HG2	1:A:280:LEU:CD2	2.50	0.42
1:B:14:LYS:HA	1:B:24:ILE:O	2.20	0.42
1:A:245:THR:HB	1:A:255:TYR:HB2	2.02	0.41
1:D:214:TYR:O	1:D:355:LEU:HD12	2.20	0.41
1:A:135:ALA:HB1	1:A:136:PRO:HD2	2.02	0.41
1:A:59:VAL:HA	1:A:150:LYS:O	2.20	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD2	1.88	0.41
1:B:236:LYS:HB3	1:B:334:THR:HB	2.01	0.41
1:A:83:LEU:HD23	1:A:83:LEU:N	2.34	0.41
1:A:32:ILE:HG23	1:A:179:HIS:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HG13	1:A:17:SER:N	2.29	0.41
1:A:253:ASP:N	1:A:253:ASP:OD1	2.54	0.41
1:B:76:GLY:H	2:C:406:PTD:HC31	1.86	0.41
1:B:330:LYS:HE2	1:B:348:ALA:HB1	2.01	0.41
1:C:67:TYR:CD2	1:C:143:CYS:HB3	2.56	0.41
1:C:250:TYR:O	2:C:405:PTD:HC31	2.19	0.41
1:C:59:VAL:HA	1:C:150:LYS:O	2.20	0.41
1:B:130:VAL:HA	1:B:295:LEU:O	2.21	0.41
1:C:12:ILE:HG13	1:C:107:LEU:HD21	2.03	0.41
1:C:197:PHE:O	1:C:198:MET:HB2	2.21	0.41
1:C:338:LEU:HD12	1:C:345:SER:OG	2.21	0.41
1:A:278:LEU:N	1:A:278:LEU:HD12	2.36	0.41
1:C:13:PHE:CE1	1:C:29:ARG:NH1	2.89	0.41
1:D:177:VAL:HG22	1:D:179:HIS:CD2	2.55	0.41
1:D:380:PHE:O	1:D:381:ALA:HB2	2.21	0.41
1:C:212:GLU:OE1	2:C:407:PTD:O5	2.38	0.41
1:C:127:PRO:HA	1:C:321:MET:CE	2.51	0.41
1:D:111:LEU:HB2	1:D:115:THR:HG21	2.03	0.41
1:B:66:ARG:CG	5:B:405:IMD:H2	2.51	0.40
1:B:330:LYS:HD2	1:B:350:GLU:CG	2.48	0.40
1:C:239:VAL:HG21	1:C:278:LEU:HD13	2.03	0.40
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.93	0.40
1:B:65:PHE:CE2	1:B:249:LEU:HB3	2.56	0.40
1:B:242:GLU:HA	1:B:257:LYS:O	2.22	0.40
1:B:332:LYS:HA	1:B:347:VAL:O	2.21	0.40
1:C:350:GLU:O	2:C:406:PTD:HC5	2.22	0.40
1:D:100:THR:HG23	1:D:104:GLN:OE1	2.22	0.40
1:A:16:ILE:CD1	1:A:20:LYS:HA	2.50	0.40
1:D:357:HIS:HB3	1:D:358:PRO:CD	2.51	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	366/414 (88%)	358 (98%)	7 (2%)	1 (0%)	44	62
1	B	342/414 (83%)	332 (97%)	9 (3%)	1 (0%)	44	62
1	C	350/414 (84%)	344 (98%)	5 (1%)	1 (0%)	44	62
1	D	338/414 (82%)	332 (98%)	6 (2%)	0	100	100
All	All	1396/1656 (84%)	1366 (98%)	27 (2%)	3 (0%)	51	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	B	35	VAL
1	C	35	VAL

5.3.2 Protein sidechains ⓘ

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	315/368 (86%)	283 (90%)	32 (10%)	8	12
1	B	287/368 (78%)	244 (85%)	43 (15%)	3	3
1	C	304/368 (83%)	282 (93%)	22 (7%)	17	26
1	D	276/368 (75%)	239 (87%)	37 (13%)	4	5
All	All	1182/1472 (80%)	1048 (89%)	134 (11%)	7	9

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	16	ILE
1	A	26	LEU
1	A	38	VAL
1	A	53	LYS
1	A	66	ARG
1	A	72	ILE
1	A	100	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	103	LEU
1	A	109	LYS
1	A	115	THR
1	A	139	VAL
1	A	189	ARG
1	A	193	SER
1	A	208	SER
1	A	209	LEU
1	A	212	GLU
1	A	232	LYS
1	A	249	LEU
1	A	251	SER
1	A	252	SER
1	A	253	ASP
1	A	274	LEU
1	A	320	VAL
1	A	338	LEU
1	A	339	LEU
1	A	345	SER
1	A	347	VAL
1	A	362	ASP
1	A	372	ASP
1	A	373	GLU
1	A	383	GLN
1	B	11	VAL
1	B	16	ILE
1	B	17	SER
1	B	24	ILE
1	B	26	LEU
1	B	38	VAL
1	B	45	VAL
1	B	46	LEU
1	B	66	ARG
1	B	69	GLN
1	B	71	ASP
1	B	72	ILE
1	B	74	VAL
1	B	86	SER
1	B	101	THR
1	B	103	LEU
1	B	119	LEU
1	B	131	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	139	VAL
1	B	154	THR
1	B	156	SER
1	B	164	ILE
1	B	170	VAL
1	B	171	ARG
1	B	172	LEU
1	B	193	SER
1	B	212	GLU
1	B	231	GLU
1	B	232	LYS
1	B	249	LEU
1	B	251	SER
1	B	252	SER
1	B	256	ILE
1	B	262	GLU
1	B	279	THR
1	B	281	VAL
1	B	287	ASN
1	B	290	ARG
1	B	293	ILE
1	B	303	ASP
1	B	343	THR
1	B	344	SER
1	B	361	GLU
1	C	10	HIS
1	C	14	LYS
1	C	26	LEU
1	C	37	ARG
1	C	38	VAL
1	C	66	ARG
1	C	90	VAL
1	C	97	SER
1	C	103	LEU
1	C	131	MET
1	C	159	VAL
1	C	170	VAL
1	C	172	LEU
1	C	189	ARG
1	C	200	ASP
1	C	212	GLU
1	C	227	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	249	LEU
1	C	266	GLU
1	C	276	LYS
1	C	320	VAL
1	C	385	LEU
1	D	17	SER
1	D	19	ASP
1	D	21	SER
1	D	26	LEU
1	D	37	ARG
1	D	38	VAL
1	D	47	VAL
1	D	56	ARG
1	D	69	GLN
1	D	71	ASP
1	D	75	MET
1	D	78	SER
1	D	86	SER
1	D	94	VAL
1	D	101	THR
1	D	103	LEU
1	D	115	THR
1	D	130	VAL
1	D	131	MET
1	D	132	LEU
1	D	168	SER
1	D	170	VAL
1	D	171	ARG
1	D	172	LEU
1	D	177	VAL
1	D	193	SER
1	D	210	SER
1	D	262	GLU
1	D	279	THR
1	D	293	ILE
1	D	303	ASP
1	D	313	LYS
1	D	320	VAL
1	D	332	LYS
1	D	336	SER
1	D	343	THR
1	D	385	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	C	178	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

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	PTD	A	405	-	6,6,6	1.84	2 (33%)	5,5,5	1.70	1 (20%)
2	PTD	A	406	-	6,6,6	1.87	2 (33%)	5,5,5	1.95	2 (40%)
2	PTD	A	407	-	6,6,6	1.82	2 (33%)	5,5,5	1.55	1 (20%)
2	PTD	A	408	-	6,6,6	1.83	2 (33%)	5,5,5	1.50	0
2	PTD	A	409	-	6,6,6	1.85	2 (33%)	5,5,5	1.69	1 (20%)
2	PTD	A	410	-	6,6,6	1.93	2 (33%)	5,5,5	1.84	2 (40%)
2	PTD	A	411	-	6,6,6	1.80	2 (33%)	5,5,5	1.68	0
2	PTD	A	412	-	6,6,6	1.83	2 (33%)	5,5,5	1.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	414	-	3,3,3	0.44	0	2,2,2	0.23	0
4	EDO	A	415	-	3,3,3	0.47	0	2,2,2	0.34	0
5	IMD	B	405	-	3,5,5	0.51	0	4,5,5	0.63	0
2	PTD	B	406	-	6,6,6	1.84	2 (33%)	5,5,5	1.67	1 (20%)
2	PTD	B	407	-	6,6,6	1.83	2 (33%)	5,5,5	1.64	0
4	EDO	B	409	-	3,3,3	0.43	0	2,2,2	0.45	0
2	PTD	C	405	-	6,6,6	1.84	2 (33%)	5,5,5	1.49	0
2	PTD	C	406	-	6,6,6	1.82	2 (33%)	5,5,5	1.52	0
2	PTD	C	407	-	6,6,6	1.85	2 (33%)	5,5,5	1.40	0
4	EDO	C	409	-	3,3,3	0.45	0	2,2,2	0.42	0
4	EDO	C	410	-	3,3,3	0.53	0	2,2,2	0.30	0
4	EDO	C	411	-	3,3,3	0.48	0	2,2,2	0.28	0
5	IMD	D	405	-	3,5,5	0.56	0	4,5,5	0.65	0
5	IMD	D	406	-	3,5,5	0.57	0	4,5,5	0.56	0
2	PTD	D	407	-	6,6,6	1.84	2 (33%)	5,5,5	1.86	2 (40%)
4	EDO	D	408	-	3,3,3	0.50	0	2,2,2	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTD	A	405	-	-	0/2/4/4	0/0/0/0
2	PTD	A	406	-	-	0/2/4/4	0/0/0/0
2	PTD	A	407	-	-	0/2/4/4	0/0/0/0
2	PTD	A	408	-	-	0/2/4/4	0/0/0/0
2	PTD	A	409	-	-	0/2/4/4	0/0/0/0
2	PTD	A	410	-	-	0/2/4/4	0/0/0/0
2	PTD	A	411	-	-	0/2/4/4	0/0/0/0
2	PTD	A	412	-	-	0/2/4/4	0/0/0/0
4	EDO	A	414	-	-	0/1/1/1	0/0/0/0
4	EDO	A	415	-	-	0/1/1/1	0/0/0/0
5	IMD	B	405	-	-	0/0/0/0	0/1/1/1
2	PTD	B	406	-	-	0/2/4/4	0/0/0/0
2	PTD	B	407	-	-	0/2/4/4	0/0/0/0
4	EDO	B	409	-	-	0/1/1/1	0/0/0/0
2	PTD	C	405	-	-	0/2/4/4	0/0/0/0
2	PTD	C	406	-	-	0/2/4/4	0/0/0/0
2	PTD	C	407	-	-	0/2/4/4	0/0/0/0
4	EDO	C	409	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	410	-	-	0/1/1/1	0/0/0/0
4	EDO	C	411	-	-	0/1/1/1	0/0/0/0
5	IMD	D	405	-	-	0/0/0/0	0/1/1/1
5	IMD	D	406	-	-	0/0/0/0	0/1/1/1
2	PTD	D	407	-	-	0/2/4/4	0/0/0/0
4	EDO	D	408	-	-	0/1/1/1	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	PTD	O1-C1	3.01	1.38	1.19
2	C	406	PTD	O1-C1	3.06	1.38	1.19
2	A	407	PTD	O1-C1	3.06	1.38	1.19
2	A	412	PTD	O1-C1	3.08	1.38	1.19
2	C	406	PTD	O5-C5	3.08	1.38	1.19
2	A	411	PTD	O5-C5	3.08	1.38	1.19
2	C	407	PTD	O5-C5	3.09	1.38	1.19
2	A	412	PTD	O5-C5	3.09	1.38	1.19
2	B	407	PTD	O5-C5	3.09	1.38	1.19
2	A	408	PTD	O5-C5	3.10	1.38	1.19
2	B	406	PTD	O5-C5	3.10	1.38	1.19
2	A	408	PTD	O1-C1	3.10	1.38	1.19
2	A	407	PTD	O5-C5	3.11	1.38	1.19
2	B	407	PTD	O1-C1	3.11	1.38	1.19
2	A	409	PTD	O1-C1	3.11	1.38	1.19
2	A	405	PTD	O1-C1	3.12	1.38	1.19
2	D	407	PTD	O1-C1	3.12	1.39	1.19
2	A	405	PTD	O5-C5	3.12	1.39	1.19
2	D	407	PTD	O5-C5	3.14	1.39	1.19
2	A	406	PTD	O5-C5	3.14	1.39	1.19
2	C	405	PTD	O1-C1	3.14	1.39	1.19
2	C	405	PTD	O5-C5	3.15	1.39	1.19
2	B	406	PTD	O1-C1	3.16	1.39	1.19
2	C	407	PTD	O1-C1	3.17	1.39	1.19
2	A	406	PTD	O1-C1	3.17	1.39	1.19
2	A	409	PTD	O5-C5	3.19	1.39	1.19
2	A	410	PTD	O1-C1	3.21	1.39	1.19
2	A	410	PTD	O5-C5	3.38	1.40	1.19

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	406	PTD	C3-C4-C5	2.06	118.68	113.05
2	A	407	PTD	C3-C2-C1	2.08	118.74	113.05
2	A	406	PTD	C3-C2-C1	2.11	118.82	113.05
2	A	410	PTD	C3-C2-C1	2.12	118.85	113.05
2	D	407	PTD	C3-C4-C5	2.21	119.10	113.05
2	A	409	PTD	C3-C4-C5	2.29	119.32	113.05
2	A	405	PTD	C3-C4-C5	2.30	119.34	113.05
2	D	407	PTD	C3-C2-C1	2.37	119.53	113.05
2	A	406	PTD	C3-C4-C5	2.66	120.32	113.05
2	A	410	PTD	C3-C4-C5	2.92	121.05	113.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	PTD	3	0
2	A	407	PTD	3	0
2	A	409	PTD	2	0
2	A	410	PTD	5	0
4	A	415	EDO	1	0
5	B	405	IMD	4	0
2	C	405	PTD	2	0
2	C	406	PTD	6	0
2	C	407	PTD	3	0
4	C	409	EDO	1	0
5	D	405	IMD	1	0
5	D	406	IMD	3	0
4	D	408	EDO	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

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, 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	369/414 (89%)	-0.08	13 (3%) 44 40	23, 42, 90, 133	0
1	B	352/414 (85%)	0.26	33 (9%) 9 7	29, 58, 120, 140	0
1	C	358/414 (86%)	-0.04	16 (4%) 34 30	25, 47, 90, 162	0
1	D	348/414 (84%)	0.21	36 (10%) 7 5	26, 52, 117, 141	0
All	All	1427/1656 (86%)	0.09	98 (6%) 18 14	23, 48, 114, 162	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	GLY	6.1
1	B	99	ALA	5.5
1	D	376	VAL	5.4
1	D	375	PHE	5.3
1	D	385	LEU	5.0
1	B	377	PHE	5.0
1	D	139	VAL	4.6
1	B	157	THR	4.6
1	B	376	VAL	4.6
1	D	186	PRO	4.4
1	B	385	LEU	4.3
1	D	51	LEU	4.3
1	A	97	SER	4.2
1	A	362	ASP	4.1
1	D	153	ALA	3.9
1	C	139	VAL	3.9
1	B	51	LEU	3.7
1	A	72	ILE	3.5
1	C	373	GLU	3.5
1	D	135	ALA	3.5
1	B	383	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	11	VAL	3.4
1	C	77	LEU	3.4
1	D	74	VAL	3.4
1	A	339	LEU	3.4
1	D	57	VAL	3.4
1	D	70	GLU	3.4
1	C	385	LEU	3.3
1	D	90	VAL	3.3
1	D	52	VAL	3.3
1	C	386	LYS	3.3
1	D	10	HIS	3.2
1	B	52	VAL	3.1
1	D	16	ILE	3.1
1	C	9	ASN	3.1
1	B	380	PHE	3.1
1	A	338	LEU	3.0
1	A	374	ASN	3.0
1	C	374	ASN	3.0
1	B	153	ALA	3.0
1	D	185	GLY	3.0
1	D	384	ASN	3.0
1	B	107	LEU	3.0
1	C	339	LEU	2.9
1	B	136	PRO	2.9
1	A	361	GLU	2.9
1	D	111	LEU	2.8
1	C	67	TYR	2.7
1	B	50	GLU	2.7
1	D	94	VAL	2.7
1	D	137	GLN	2.7
1	B	164	ILE	2.7
1	A	372	ASP	2.6
1	C	97	SER	2.6
1	C	69	GLN	2.6
1	C	362	ASP	2.6
1	A	386	LYS	2.6
1	D	9	ASN	2.6
1	B	55	LYS	2.5
1	D	107	LEU	2.5
1	D	53	LYS	2.5
1	D	138	ASP	2.5
1	D	91	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	135	ALA	2.5
1	C	98	GLY	2.4
1	D	50	GLU	2.4
1	B	290	ARG	2.4
1	D	136	PRO	2.4
1	A	98	GLY	2.4
1	D	360	PRO	2.3
1	D	56	ARG	2.3
1	D	187	GLN	2.3
1	B	54	GLY	2.2
1	C	136	PRO	2.2
1	B	338	LEU	2.2
1	B	115	THR	2.2
1	C	250	TYR	2.2
1	D	183	ASP	2.2
1	B	379	GLU	2.2
1	A	137	GLN	2.2
1	A	385	LEU	2.1
1	D	54	GLY	2.1
1	B	95	GLY	2.1
1	B	158	ASP	2.1
1	B	156	SER	2.1
1	B	56	ARG	2.1
1	B	57	VAL	2.1
1	B	74	VAL	2.1
1	B	155	HIS	2.1
1	D	55	LYS	2.1
1	B	286	ASN	2.1
1	D	382	ARG	2.1
1	B	111	LEU	2.1
1	D	383	GLN	2.1
1	D	106	SER	2.1
1	B	154	THR	2.0
1	A	139	VAL	2.0
1	B	315	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	PTD	C	407	7/7	0.85	0.30	13.65	57,64,71,76	0
4	EDO	B	409	4/4	0.88	0.33	8.60	55,60,61,70	0
2	PTD	A	411	7/7	0.79	0.29	5.79	65,71,75,77	0
2	PTD	A	406	7/7	0.94	0.32	5.70	27,35,36,38	0
2	PTD	A	410	7/7	0.81	0.36	5.60	55,56,62,63	0
4	EDO	C	409	4/4	0.89	0.27	5.13	58,59,63,65	0
6	K	C	408	1/1	0.93	0.28	4.49	88,88,88,88	0
5	IMD	D	406	5/5	0.96	0.25	2.96	80,81,88,91	0
5	IMD	D	405	5/5	0.96	0.22	2.84	72,73,74,75	0
2	PTD	A	408	7/7	0.88	0.20	2.59	68,70,72,72	0
5	IMD	B	405	5/5	0.86	0.26	2.56	86,89,89,89	0
2	PTD	C	406	7/7	0.86	0.32	2.44	60,63,84,92	0
4	EDO	D	408	4/4	0.93	0.39	2.34	62,63,63,63	0
2	PTD	C	405	7/7	0.67	0.33	2.27	69,72,76,77	0
4	EDO	C	411	4/4	0.97	0.23	2.27	60,65,78,85	0
2	PTD	A	405	7/7	0.91	0.24	1.97	42,48,72,75	0
4	EDO	A	414	4/4	0.98	0.24	1.93	36,39,41,49	0
2	PTD	A	407	7/7	0.64	0.26	1.40	62,70,78,82	0
2	PTD	B	406	7/7	0.78	0.20	1.29	69,73,81,83	0
2	PTD	A	409	7/7	0.88	0.21	0.39	45,54,76,77	0
4	EDO	C	410	4/4	0.99	0.18	-0.09	26,30,37,38	0
2	PTD	A	412	7/7	0.84	0.22	-	59,63,72,72	0
2	PTD	D	407	7/7	0.88	0.20	-	52,61,69,69	0
3	NA	B	408	1/1	0.93	0.37	-	45,45,45,45	0
2	PTD	B	407	7/7	0.84	0.23	-	62,65,71,74	0
4	EDO	A	415	4/4	0.93	0.23	-	59,63,64,68	0
3	NA	A	413	1/1	0.96	0.23	-	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.