Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 03:11 pm GMT

PDB ID	:	7ZPF
Title	:	Three-dimensional structure of AIP56, a short-trip single chain AB toxin from Photobacterium damselae subsp. piscicida.
Authors	:	Lisboa, J.; Pereira, P.J.B.; dos Santos, N.M.S.
Deposited on	:	2022-04-27
Resolution	:	2.54 Å(reported)

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

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

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

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

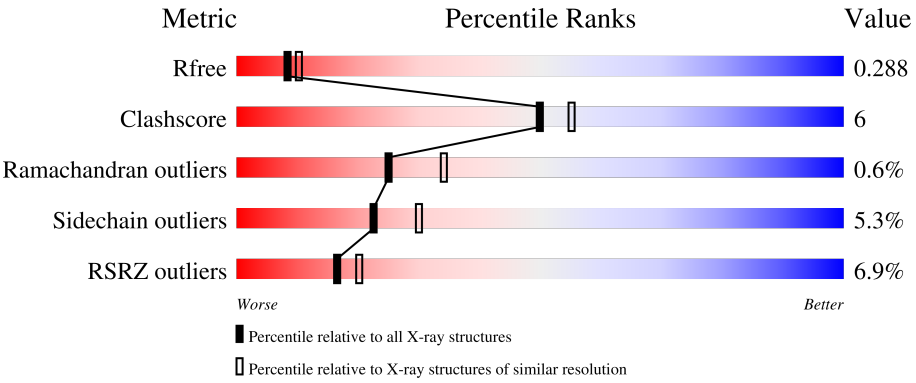
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	521	3% 75% 13% • 11%
1	B	521	4% 72% 14% • 13%
1	C	521	9% 71% 13% • 15%
1	D	521	8% 73% 12% • 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14880 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 Aip56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3745	2380	644	715	6			
1	B	452	Total	C	N	O	S	0	0	0
			3662	2331	629	696	6			
1	C	445	Total	C	N	O	S	0	0	0
			3599	2291	621	681	6			
1	D	449	Total	C	N	O	S	0	0	0
			3629	2306	624	693	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP Q2VL32
A	499	GLU	-	expression tag	UNP Q2VL32
A	500	HIS	-	expression tag	UNP Q2VL32
A	501	HIS	-	expression tag	UNP Q2VL32
A	502	HIS	-	expression tag	UNP Q2VL32
A	503	HIS	-	expression tag	UNP Q2VL32
A	504	HIS	-	expression tag	UNP Q2VL32
A	505	HIS	-	expression tag	UNP Q2VL32
B	498	LEU	-	expression tag	UNP Q2VL32
B	499	GLU	-	expression tag	UNP Q2VL32
B	500	HIS	-	expression tag	UNP Q2VL32
B	501	HIS	-	expression tag	UNP Q2VL32
B	502	HIS	-	expression tag	UNP Q2VL32
B	503	HIS	-	expression tag	UNP Q2VL32
B	504	HIS	-	expression tag	UNP Q2VL32
B	505	HIS	-	expression tag	UNP Q2VL32
C	498	LEU	-	expression tag	UNP Q2VL32
C	499	GLU	-	expression tag	UNP Q2VL32
C	500	HIS	-	expression tag	UNP Q2VL32
C	501	HIS	-	expression tag	UNP Q2VL32
C	502	HIS	-	expression tag	UNP Q2VL32

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Chain	Residue	Modelled	Actual	Comment	Reference
C	503	HIS	-	expression tag	UNP Q2VL32
C	504	HIS	-	expression tag	UNP Q2VL32
C	505	HIS	-	expression tag	UNP Q2VL32
D	498	LEU	-	expression tag	UNP Q2VL32
D	499	GLU	-	expression tag	UNP Q2VL32
D	500	HIS	-	expression tag	UNP Q2VL32
D	501	HIS	-	expression tag	UNP Q2VL32
D	502	HIS	-	expression tag	UNP Q2VL32
D	503	HIS	-	expression tag	UNP Q2VL32
D	504	HIS	-	expression tag	UNP Q2VL32
D	505	HIS	-	expression tag	UNP Q2VL32

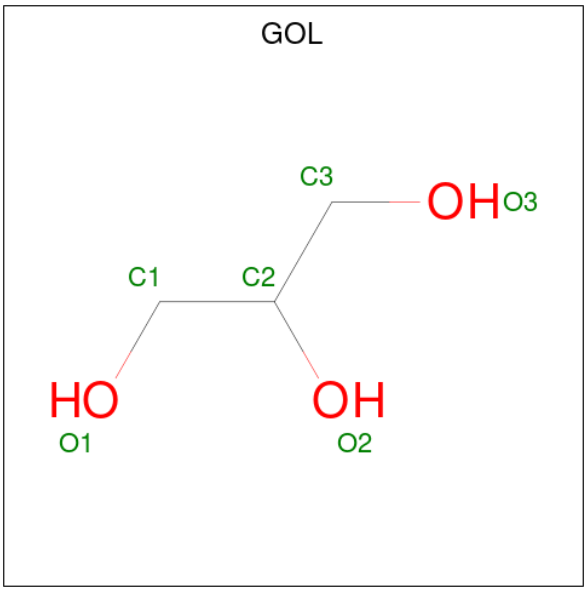
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	D	2	Total Ni 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

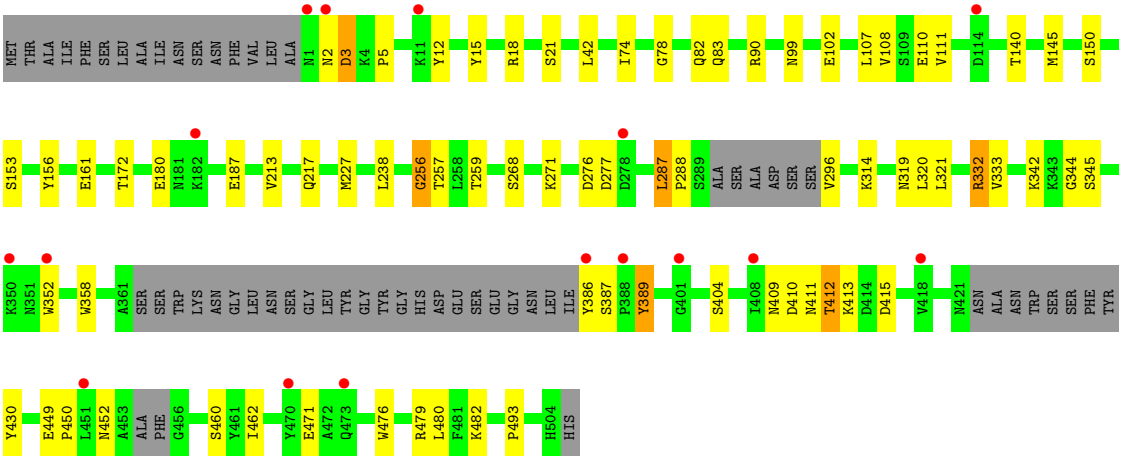
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0
5	B	69	Total O 69 69	0	0
5	C	43	Total O 43 43	0	0
5	D	30	Total O 30 30	0	0

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.

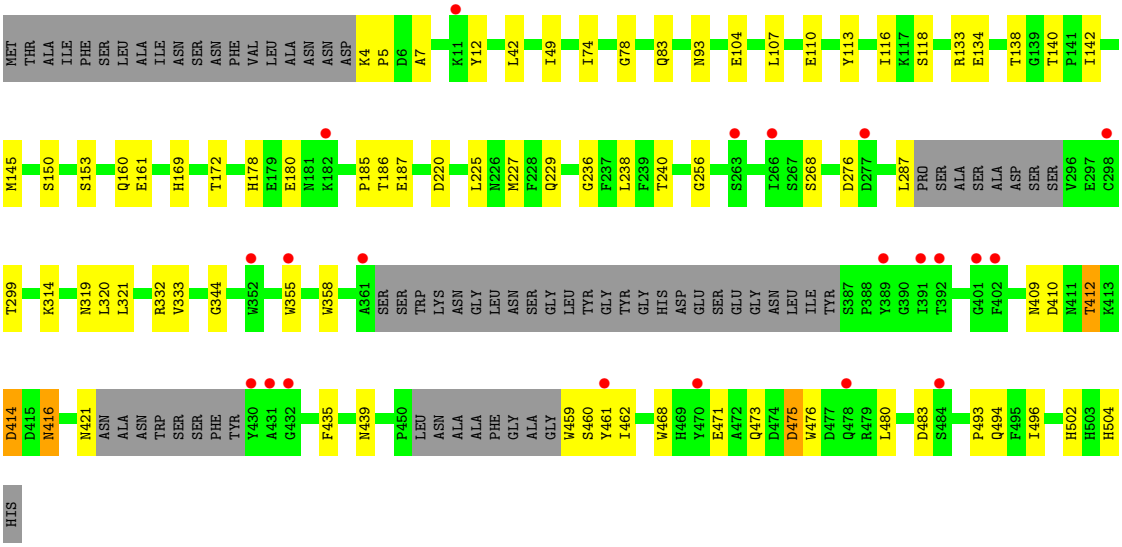
• Molecule 1: Aip56

Chain A:



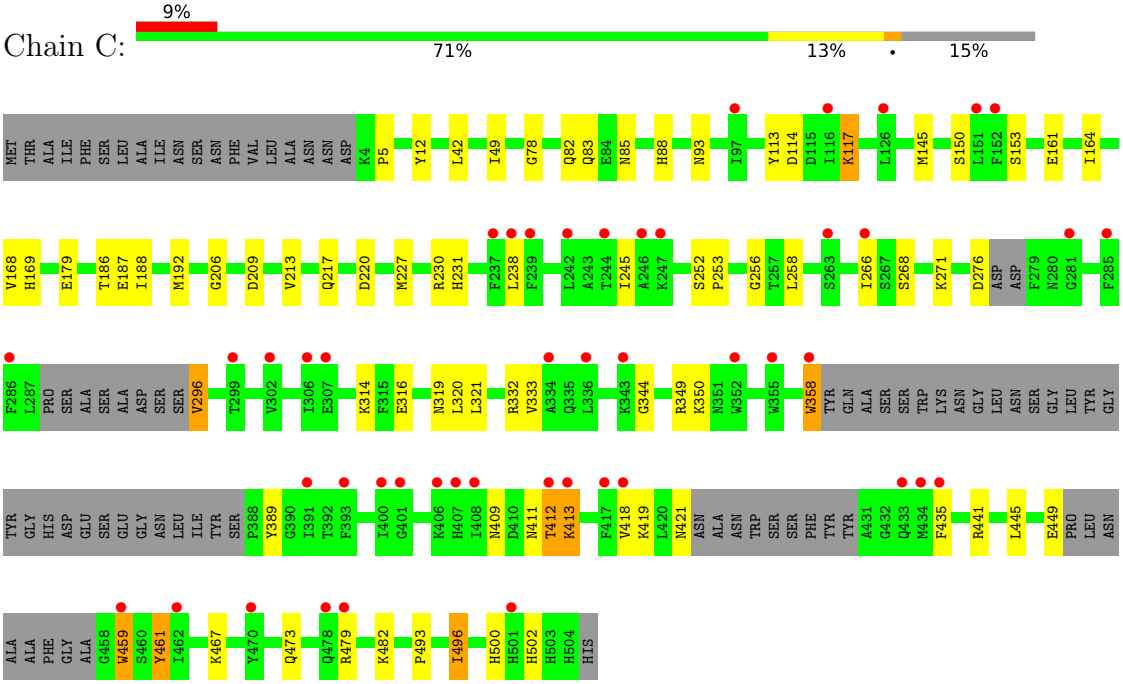
• Molecule 1: Aip56

Chain B:



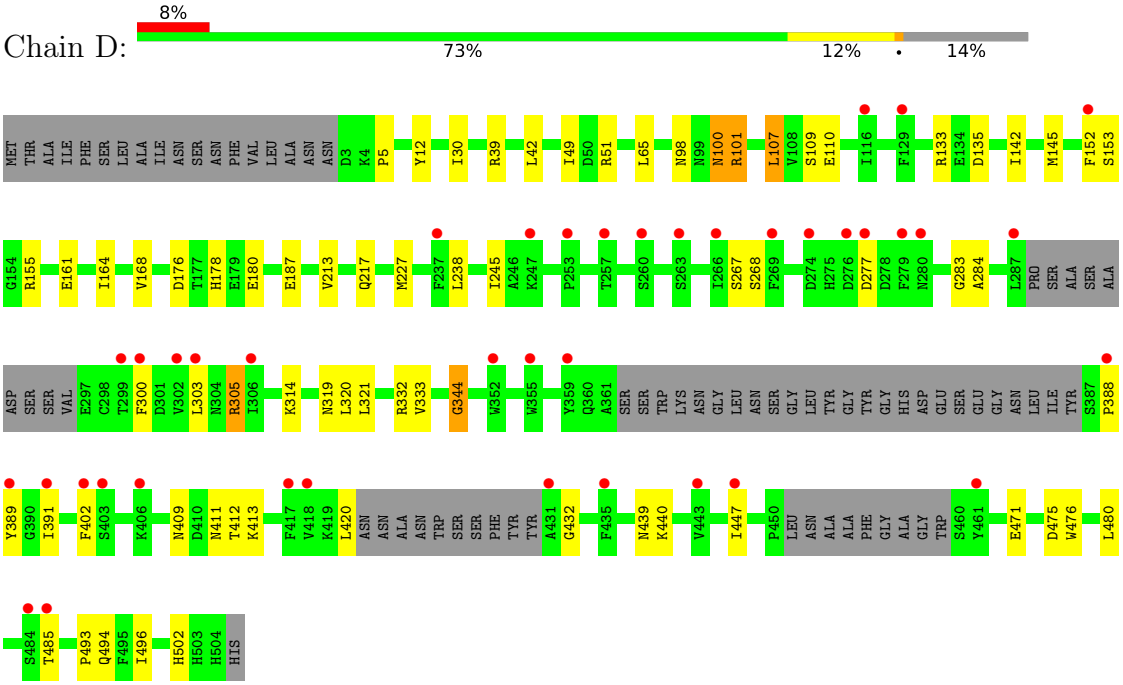
• Molecule 1: Aip56

Chain C:



• Molecule 1: Aip56

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.13Å 193.85Å 91.62Å 90.00° 113.24° 90.00°	Depositor
Resolution (Å)	46.28 – 2.54 46.28 – 2.54	Depositor EDS
% Data completeness (in resolution range)	69.6 (46.28-2.54) 69.4 (46.28-2.54)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.4, PHENIX 1.20	Depositor
R, R_{free}	0.240 , 0.282 0.236 , 0.288	Depositor DCC
R_{free} test set	2563 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14880	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.38% 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: ZN, GOL, NI

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	0/3850	0.60	0/5221
1	B	0.43	0/3765	0.59	0/5104
1	C	0.42	0/3698	0.59	0/5008
1	D	0.43	0/3729	0.61	0/5053
All	All	0.43	0/15042	0.60	0/20386

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	3745	0	3519	46	0
1	B	3662	0	3446	49	0
1	C	3599	0	3398	42	0
1	D	3629	0	3416	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	6	0	8	1	0
4	B	24	0	32	3	0
5	A	65	0	0	1	0
5	B	69	0	0	2	0
5	C	43	0	0	1	0
5	D	30	0	0	2	0
All	All	14880	0	13819	164	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 (164) 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:B:462:ILE:HD13	1:B:471:GLU:HG3	1.62	0.81
1:A:332:ARG:HB2	5:A:701:HOH:O	1.82	0.78
1:B:138:THR:OG1	1:B:140:THR:HG22	1.85	0.77
1:A:476:TRP:HA	1:A:479:ARG:HG3	1.67	0.77
1:A:389:TYR:H	1:A:389:TYR:HD2	1.33	0.76
1:D:496:ILE:HD13	1:D:502:HIS:NE2	2.03	0.74
1:A:259:THR:CG2	1:B:240:THR:HG21	2.17	0.73
1:A:476:TRP:O	1:A:480:LEU:HB2	1.88	0.73
1:B:116:ILE:HG22	1:B:225:LEU:HD21	1.72	0.71
1:A:333:VAL:HG22	1:A:412:THR:HG23	1.75	0.69
1:C:231:HIS:ND1	1:C:238:LEU:HD13	2.07	0.68
1:B:160:GLN:HE22	4:B:604:GOL:H32	1.57	0.68
1:C:409:ASN:H	1:C:412:THR:HG22	1.59	0.68
1:C:459:TRP:CD1	1:C:459:TRP:N	2.61	0.67
1:B:409:ASN:H	1:B:412:THR:HG22	1.59	0.67
1:C:114:ASP:HA	1:C:117:LYS:HE2	1.77	0.67
1:A:259:THR:HG21	1:B:240:THR:HG21	1.78	0.66
1:B:220:ASP:HB3	5:B:722:HOH:O	1.95	0.66
1:B:496:ILE:HD13	1:B:502:HIS:NE2	2.12	0.65
1:D:471:GLU:HG2	1:D:476:TRP:HB3	1.81	0.63
1:D:176:ASP:OD1	5:D:701:HOH:O	2.15	0.63
1:A:409:ASN:H	1:A:412:THR:HG22	1.64	0.61
1:A:449:GLU:HB2	1:A:450:PRO:HD2	1.81	0.61
1:C:459:TRP:N	1:C:459:TRP:HD1	1.98	0.61
1:A:321:LEU:HD11	1:A:493:PRO:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ILE:HD13	1:A:471:GLU:HG3	1.81	0.61
1:C:413:LYS:NZ	1:C:419:LYS:HG2	2.16	0.60
1:B:113:TYR:H	4:B:603:GOL:H31	1.66	0.60
1:C:321:LEU:HD11	1:C:493:PRO:HB3	1.83	0.60
1:D:133:ARG:HG3	1:D:142:ILE:HB	1.84	0.60
1:D:314:LYS:HB3	1:D:320:LEU:HD23	1.84	0.60
1:D:321:LEU:HD11	1:D:493:PRO:HB3	1.83	0.59
1:C:314:LYS:HB3	1:C:320:LEU:HD23	1.84	0.59
1:B:5:PRO:HG2	1:B:12:TYR:HA	1.85	0.59
1:C:413:LYS:HZ3	1:C:419:LYS:HG2	1.66	0.59
1:B:321:LEU:HD11	1:B:493:PRO:HB3	1.84	0.59
1:C:473:GLN:HE22	1:C:479:ARG:HH22	1.51	0.59
1:A:257:THR:HA	1:B:240:THR:OG1	2.03	0.58
1:A:404:SER:HB3	1:A:430:TYR:HB2	1.86	0.58
1:C:473:GLN:NE2	1:C:479:ARG:HH22	2.02	0.58
1:A:2:ASN:ND2	1:A:18:ARG:NH1	2.52	0.57
1:A:314:LYS:HB3	1:A:320:LEU:HD23	1.86	0.57
1:B:416:ASN:HD22	1:B:468:TRP:H	1.53	0.56
1:B:460:SER:HB2	1:B:476:TRP:CH2	2.40	0.56
1:A:108:VAL:O	1:A:111:VAL:HG12	2.06	0.55
1:B:314:LYS:HB3	1:B:320:LEU:HD23	1.87	0.55
1:C:231:HIS:HE1	1:C:258:LEU:HD13	1.71	0.55
1:C:113:TYR:O	1:C:117:LYS:HG3	2.07	0.54
1:A:2:ASN:ND2	1:A:18:ARG:HH11	2.05	0.54
1:D:164:ILE:O	1:D:168:VAL:HG23	2.09	0.53
1:D:439:ASN:O	1:D:494:GLN:HG2	2.08	0.53
1:C:413:LYS:HZ3	1:C:419:LYS:CG	2.21	0.53
1:A:156:TYR:OH	4:A:603:GOL:O3	2.25	0.53
1:C:496:ILE:HD13	1:C:502:HIS:NE2	2.24	0.53
1:A:161:GLU:OE1	1:A:187:GLU:OE1	2.27	0.53
1:A:287:LEU:HD13	1:A:288:PRO:HD2	1.90	0.53
1:B:178:HIS:CD2	1:B:178:HIS:H	2.27	0.53
1:A:352:TRP:NE1	1:A:358:TRP:CE3	2.77	0.52
1:A:259:THR:HG23	1:B:240:THR:HG21	1.91	0.52
1:B:462:ILE:HD13	1:B:471:GLU:CG	2.38	0.52
1:B:169:HIS:CE1	1:B:186:THR:HG21	2.45	0.52
1:B:459:TRP:HZ3	1:B:461:TYR:HH	1.56	0.52
1:D:409:ASN:O	1:D:413:LYS:HB3	2.09	0.52
1:D:135:ASP:HB2	1:D:142:ILE:HD11	1.92	0.51
1:C:230:ARG:HG3	1:C:231:HIS:HD2	1.75	0.51
1:D:476:TRP:HB2	1:D:480:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:MET:SD	1:B:238:LEU:HD21	2.51	0.51
1:B:287:LEU:HD23	1:B:299:THR:HB	1.93	0.51
1:A:352:TRP:CD1	1:A:358:TRP:HE3	2.29	0.51
1:D:107:LEU:HD23	1:D:110:GLU:HG3	1.93	0.51
1:B:160:GLN:NE2	4:B:604:GOL:H32	2.25	0.50
1:A:462:ILE:HD11	1:A:476:TRP:CD2	2.46	0.50
1:D:284:ALA:HB2	1:D:305:ARG:HH11	1.76	0.50
1:D:51:ARG:NH2	1:D:300:PHE:CE1	2.80	0.50
1:A:227:MET:SD	1:A:238:LEU:HD21	2.53	0.49
1:A:476:TRP:HA	1:A:479:ARG:HE	1.77	0.49
1:A:107:LEU:HB2	1:A:110:GLU:HG3	1.95	0.49
1:B:118:SER:HB3	1:D:267:SER:HB3	1.95	0.49
1:D:333:VAL:HG22	1:D:412:THR:CG2	2.43	0.49
1:B:225:LEU:HB3	1:D:152:PHE:HB3	1.95	0.48
1:D:51:ARG:NH2	1:D:300:PHE:HE1	2.11	0.48
1:A:99:ASN:ND2	1:A:102:GLU:OE2	2.46	0.48
1:A:352:TRP:NE1	1:A:358:TRP:HE3	2.12	0.48
1:B:355:TRP:HB2	1:B:435:PHE:CD2	2.49	0.48
1:D:5:PRO:HG2	1:D:12:TYR:HA	1.95	0.48
1:D:178:HIS:H	1:D:178:HIS:CD2	2.30	0.48
1:B:502:HIS:HD2	5:B:719:HOH:O	1.96	0.48
1:C:266:ILE:HG12	1:C:296:VAL:HG11	1.96	0.48
1:C:413:LYS:NZ	1:C:419:LYS:CG	2.77	0.48
1:A:256:GLY:HA3	1:B:236:GLY:HA3	1.96	0.48
1:C:231:HIS:CE1	1:C:238:LEU:HD13	2.49	0.48
1:C:358:TRP:C	1:C:358:TRP:CD1	2.87	0.48
1:D:409:ASN:HB3	1:D:412:THR:HB	1.96	0.47
1:D:321:LEU:CD1	1:D:493:PRO:HB3	2.44	0.47
1:A:476:TRP:HA	1:A:479:ARG:CG	2.42	0.47
1:C:164:ILE:O	1:C:168:VAL:HG23	2.13	0.47
1:C:227:MET:SD	1:C:238:LEU:HD21	2.54	0.47
1:B:321:LEU:CD1	1:B:493:PRO:HB3	2.44	0.47
1:A:150:SER:HB3	1:A:153:SER:HB3	1.97	0.47
1:D:161:GLU:OE2	1:D:187:GLU:OE2	2.32	0.47
1:A:321:LEU:CD1	1:A:493:PRO:HB3	2.43	0.47
1:B:225:LEU:HD13	1:D:152:PHE:CG	2.49	0.47
1:C:321:LEU:CD1	1:C:493:PRO:HB3	2.44	0.47
1:B:150:SER:HB3	1:B:153:SER:HB3	1.96	0.47
1:D:440:LYS:HG2	1:D:496:ILE:HA	1.98	0.46
1:D:227:MET:SD	1:D:238:LEU:HD21	2.55	0.46
1:B:333:VAL:HG22	1:B:412:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLN:HG3	1:D:153:SER:HA	1.96	0.45
1:C:188:ILE:O	1:C:192:MET:HG3	2.17	0.45
1:B:4:LYS:N	1:B:5:PRO:HD3	2.31	0.45
1:C:169:HIS:CE1	1:C:186:THR:HG21	2.52	0.45
1:D:344:GLY:HA3	1:D:388:PRO:HD2	1.99	0.45
1:D:391:ILE:HD13	5:D:702:HOH:O	2.17	0.45
1:D:333:VAL:HG22	1:D:412:THR:HG22	2.00	0.44
1:D:213:VAL:O	1:D:217:GLN:HG3	2.18	0.44
1:A:213:VAL:O	1:A:217:GLN:HG3	2.17	0.44
1:A:74:ILE:HG23	1:A:172:THR:CG2	2.48	0.44
1:B:107:LEU:HB2	1:B:110:GLU:HG3	2.00	0.44
1:A:345:SER:OG	1:A:387:SER:HB2	2.18	0.44
1:A:5:PRO:HG2	1:A:12:TYR:HA	2.00	0.43
1:B:74:ILE:HG23	1:B:172:THR:CG2	2.49	0.43
1:C:220:ASP:HB3	5:C:711:HOH:O	2.18	0.43
1:C:5:PRO:HG2	1:C:12:TYR:HA	2.00	0.43
1:B:332:ARG:CZ	1:B:414:ASP:HB2	2.49	0.43
1:B:473:GLN:HB3	1:B:475:ASP:OD2	2.18	0.43
1:C:161:GLU:OE1	1:C:187:GLU:OE2	2.36	0.43
1:D:107:LEU:HD21	1:D:109:SER:HB2	2.00	0.42
1:B:439:ASN:O	1:B:494:GLN:HG2	2.19	0.42
1:A:389:TYR:HD2	1:A:389:TYR:N	2.08	0.42
1:B:161:GLU:OE2	1:B:187:GLU:OE2	2.37	0.42
1:C:150:SER:HB3	1:C:153:SER:HB3	2.01	0.42
1:C:213:VAL:O	1:C:217:GLN:HG3	2.19	0.42
1:C:413:LYS:HG2	1:C:418:VAL:HG11	2.02	0.42
1:D:402:PHE:HB3	1:D:432:GLY:O	2.20	0.42
1:B:7:ALA:O	1:B:185:PRO:HG3	2.19	0.42
1:B:358:TRP:CD1	1:B:435:PHE:HE2	2.37	0.42
1:B:78:GLY:HA2	1:B:83:GLN:HB2	2.01	0.42
1:C:206:GLY:H	1:C:209:ASP:HB2	1.85	0.42
1:D:98:ASN:HB3	1:D:101:ARG:HG2	2.01	0.42
1:A:352:TRP:CD1	1:A:358:TRP:CE3	3.07	0.42
1:C:49:ILE:HD13	1:C:245:ILE:HD12	2.02	0.42
1:C:252:SER:HA	1:C:253:PRO:HD3	1.97	0.42
1:B:49:ILE:HG13	1:B:93:ASN:CB	2.50	0.42
1:C:78:GLY:HA2	1:C:83:GLN:HB2	2.01	0.42
1:D:30:ILE:HG23	1:D:65:LEU:HG	2.02	0.41
1:D:49:ILE:HD13	1:D:245:ILE:HD12	2.02	0.41
1:C:85:ASN:HB3	1:C:88:HIS:CG	2.56	0.41
1:D:100:ASN:HB2	1:D:101:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:GLU:OE1	1:C:441:ARG:NH2	2.54	0.41
1:A:3:ASP:O	1:A:5:PRO:HD3	2.20	0.41
1:B:133:ARG:HG2	1:B:134:GLU:N	2.35	0.41
1:C:333:VAL:HG22	1:C:412:THR:HG23	2.02	0.41
1:A:140:THR:HG22	1:C:500:HIS:ND1	2.35	0.41
1:C:49:ILE:HG12	1:C:93:ASN:CB	2.51	0.41
1:A:78:GLY:HA2	1:A:83:GLN:HB2	2.02	0.41
1:A:333:VAL:CG2	1:A:412:THR:HG23	2.48	0.41
1:B:4:LYS:N	1:B:5:PRO:CD	2.84	0.41
1:B:416:ASN:HD22	1:B:468:TRP:N	2.17	0.41
1:C:117:LYS:HG3	1:C:117:LYS:H	1.67	0.41
1:C:445:LEU:HD23	1:C:461:TYR:CD2	2.54	0.41
1:B:476:TRP:HB2	1:B:480:LEU:HD22	2.02	0.40
1:A:5:PRO:HD2	1:A:15:TYR:CD2	2.55	0.40
1:A:409:ASN:O	1:A:413:LYS:HB2	2.22	0.40
1:A:460:SER:CB	1:A:476:TRP:HE1	2.33	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	454/521 (87%)	427 (94%)	25 (6%)	2 (0%)	34	46
1	B	442/521 (85%)	420 (95%)	19 (4%)	3 (1%)	22	30
1	C	433/521 (83%)	408 (94%)	22 (5%)	3 (1%)	22	30
1	D	439/521 (84%)	414 (94%)	23 (5%)	2 (0%)	29	40
All	All	1768/2084 (85%)	1669 (94%)	89 (5%)	10 (1%)	25	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	256	GLY
1	D	283	GLY
1	A	256	GLY
1	B	344	GLY
1	B	416	ASN
1	A	344	GLY
1	C	496	ILE
1	B	256	GLY
1	C	344	GLY
1	D	344	GLY

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	403/448 (90%)	379 (94%)	24 (6%)	19	25
1	B	395/448 (88%)	380 (96%)	15 (4%)	33	45
1	C	388/448 (87%)	363 (94%)	25 (6%)	17	23
1	D	392/448 (88%)	372 (95%)	20 (5%)	24	32
All	All	1578/1792 (88%)	1494 (95%)	84 (5%)	22	30

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	21	SER
1	A	42	LEU
1	A	82	GLN
1	A	90	ARG
1	A	145	MET
1	A	180	GLU
1	A	268	SER
1	A	271	LYS
1	A	276	ASP
1	A	277	ASP
1	A	287	LEU

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Mol	Chain	Res	Type
1	A	296	VAL
1	A	319	ASN
1	A	332	ARG
1	A	342	LYS
1	A	386	TYR
1	A	389	TYR
1	A	410	ASP
1	A	411	ASN
1	A	412	THR
1	A	415	ASP
1	A	452	ASN
1	A	482	LYS
1	B	42	LEU
1	B	104	GLU
1	B	142	ILE
1	B	145	MET
1	B	180	GLU
1	B	268	SER
1	B	276	ASP
1	B	319	ASN
1	B	410	ASP
1	B	412	THR
1	B	414	ASP
1	B	421	ASN
1	B	475	ASP
1	B	483	ASP
1	B	504	HIS
1	C	42	LEU
1	C	82	GLN
1	C	117	LYS
1	C	145	MET
1	C	179	GLU
1	C	268	SER
1	C	271	LYS
1	C	276	ASP
1	C	296	VAL
1	C	319	ASN
1	C	332	ARG
1	C	349	ARG
1	C	350	LYS
1	C	358	TRP
1	C	389	TYR

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Mol	Chain	Res	Type
1	C	411	ASN
1	C	412	THR
1	C	413	LYS
1	C	421	ASN
1	C	435	PHE
1	C	449	GLU
1	C	459	TRP
1	C	461	TYR
1	C	467	LYS
1	C	482	LYS
1	D	39	ARG
1	D	42	LEU
1	D	100	ASN
1	D	101	ARG
1	D	107	LEU
1	D	145	MET
1	D	155	ARG
1	D	180	GLU
1	D	268	SER
1	D	277	ASP
1	D	303	LEU
1	D	305	ARG
1	D	319	ASN
1	D	332	ARG
1	D	389	TYR
1	D	411	ASN
1	D	420	LEU
1	D	447	ILE
1	D	475	ASP
1	D	485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	183	GLN
1	A	394	ASN
1	A	501	HIS
1	B	122	GLN
1	B	178	HIS
1	B	183	GLN
1	B	319	ASN

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Mol	Chain	Res	Type
1	B	394	ASN
1	B	416	ASN
1	C	183	GLN
1	C	330	ASN
1	C	394	ASN
1	C	421	ASN
1	C	473	GLN
1	D	122	GLN
1	D	178	HIS
1	D	183	GLN
1	D	360	GLN
1	D	394	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	GOL	B	604	-	5,5,5	0.15	0	5,5,5	0.30	0
4	GOL	A	603	-	5,5,5	0.28	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	B	603	-	5,5,5	0.09	0	5,5,5	0.28	0
4	GOL	B	605	-	5,5,5	0.10	0	5,5,5	0.21	0
4	GOL	B	602	-	5,5,5	0.11	0	5,5,5	0.21	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
4	GOL	B	604	-	-	2/4/4/4	-
4	GOL	A	603	-	-	2/4/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-
4	GOL	B	602	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
4	B	604	GOL	C1-C2-C3-O3
4	B	604	GOL	O2-C2-C3-O3
4	A	603	GOL	O1-C1-C2-O2
4	B	602	GOL	C1-C2-C3-O3
4	B	603	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	GOL	2	0
4	A	603	GOL	1	0
4	B	603	GOL	1	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, 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	464/521 (89%)	0.28	16 (3%) 45 52	25, 56, 88, 109	0
1	B	452/521 (86%)	0.36	21 (4%) 32 39	24, 56, 87, 98	0
1	C	445/521 (85%)	0.68	47 (10%) 6 8	37, 76, 126, 142	0
1	D	449/521 (86%)	0.57	40 (8%) 9 11	30, 66, 109, 117	0
All	All	1810/2084 (86%)	0.47	124 (6%) 16 20	24, 62, 110, 142	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	417	PHE	7.6
1	D	300	PHE	5.7
1	C	352	TRP	5.6
1	C	355	TRP	5.3
1	D	263	SER	5.3
1	C	413	LYS	5.0
1	C	285	PHE	4.9
1	C	435	PHE	4.8
1	A	408	ILE	4.6
1	C	307	GLU	4.6
1	B	401	GLY	4.4
1	D	355	TRP	4.3
1	A	386	TYR	4.3
1	C	306	ILE	4.1
1	D	431	ALA	4.1
1	D	303	LEU	3.9
1	D	302	VAL	3.9
1	D	461	TYR	3.9
1	D	402	PHE	3.8
1	C	418	VAL	3.8
1	C	433	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	451	LEU	3.8
1	D	352	TRP	3.7
1	D	247	LYS	3.7
1	C	406	LYS	3.6
1	C	116	ILE	3.6
1	D	116	ILE	3.6
1	D	276	ASP	3.6
1	C	237	PHE	3.5
1	C	401	GLY	3.5
1	B	389	TYR	3.4
1	D	279	PHE	3.4
1	A	278	ASP	3.4
1	D	435	PHE	3.3
1	C	266	ILE	3.2
1	B	461	TYR	3.2
1	C	408	ILE	3.2
1	D	280	ASN	3.2
1	B	432	GLY	3.2
1	D	257	THR	3.1
1	D	417	PHE	3.1
1	C	391	ILE	3.0
1	B	484	SER	3.0
1	D	403	SER	3.0
1	D	359	TYR	3.0
1	A	352	TRP	3.0
1	D	269	PHE	2.9
1	C	247	LYS	2.9
1	C	97	ILE	2.9
1	A	470	TYR	2.9
1	C	242	LEU	2.9
1	C	407	HIS	2.9
1	B	361	ALA	2.9
1	C	358	TRP	2.9
1	D	299	THR	2.9
1	C	281	GLY	2.8
1	C	434	MET	2.8
1	C	246	ALA	2.8
1	A	473	GLN	2.7
1	B	470	TYR	2.7
1	B	392	THR	2.7
1	D	274	ASP	2.7
1	C	336	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	114	ASP	2.6
1	B	402	PHE	2.6
1	C	286	PHE	2.5
1	C	400	ILE	2.5
1	B	430	TYR	2.5
1	C	299	THR	2.5
1	C	239	PHE	2.5
1	C	151	LEU	2.5
1	B	266	ILE	2.5
1	C	462	ILE	2.5
1	C	343	LYS	2.4
1	C	479	ARG	2.4
1	B	277	ASP	2.4
1	B	391	ILE	2.4
1	D	388	PRO	2.4
1	A	11	LYS	2.4
1	C	152	PHE	2.4
1	D	418	VAL	2.4
1	B	478	GLN	2.3
1	C	470	TYR	2.3
1	C	334	ALA	2.3
1	D	266	ILE	2.3
1	C	244	THR	2.3
1	C	412	THR	2.3
1	D	277	ASP	2.3
1	D	389	TYR	2.3
1	C	302	VAL	2.3
1	A	401	GLY	2.3
1	B	263	SER	2.3
1	C	393	PHE	2.3
1	C	501	HIS	2.3
1	D	253	PRO	2.2
1	A	2	ASN	2.2
1	D	485	THR	2.2
1	A	388	PRO	2.2
1	D	484	SER	2.2
1	B	355	TRP	2.2
1	D	152	PHE	2.1
1	B	11	LYS	2.1
1	A	418	VAL	2.1
1	D	287	LEU	2.1
1	C	263	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	182	LYS	2.1
1	D	443	VAL	2.1
1	C	478	GLN	2.1
1	D	306	ILE	2.1
1	D	447	ILE	2.1
1	B	352	TRP	2.1
1	D	406	LYS	2.1
1	C	126	LEU	2.1
1	A	1	ASN	2.1
1	C	459	TRP	2.1
1	B	431	ALA	2.0
1	D	260	SER	2.0
1	C	238	LEU	2.0
1	D	129	PHE	2.0
1	B	298	CYS	2.0
1	D	391	ILE	2.0
1	D	237	PHE	2.0
1	B	182	LYS	2.0
1	A	350	LYS	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
4	GOL	B	605	6/6	0.79	0.17	72,72,72,72	0
4	GOL	B	603	6/6	0.91	0.16	51,51,52,52	0
4	GOL	B	602	6/6	0.94	0.12	59,59,59,59	0
4	GOL	B	604	6/6	0.95	0.15	54,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	603	6/6	0.95	0.17	43,44,44,44	0
2	ZN	B	601	1/1	0.99	0.15	40,40,40,40	0
2	ZN	D	601	1/1	0.99	0.18	44,44,44,44	0
3	NI	C	602	1/1	0.99	0.16	54,54,54,54	0
3	NI	D	602	1/1	0.99	0.17	48,48,48,48	0
3	NI	D	603	1/1	0.99	0.15	49,49,49,49	0
3	NI	A	602	1/1	1.00	0.15	38,38,38,38	0
2	ZN	C	601	1/1	1.00	0.15	50,50,50,50	0
2	ZN	A	601	1/1	1.00	0.19	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.