Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:57 pm BST

PDB ID	:	6NAL
Title	:	Crystal Structure of Gram Negative Toxin
Authors	:	Morton, C.J.; Lawrence, S.A.; Parker, M.W.
Deposited on	:	2018-12-05
Resolution	:	2.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

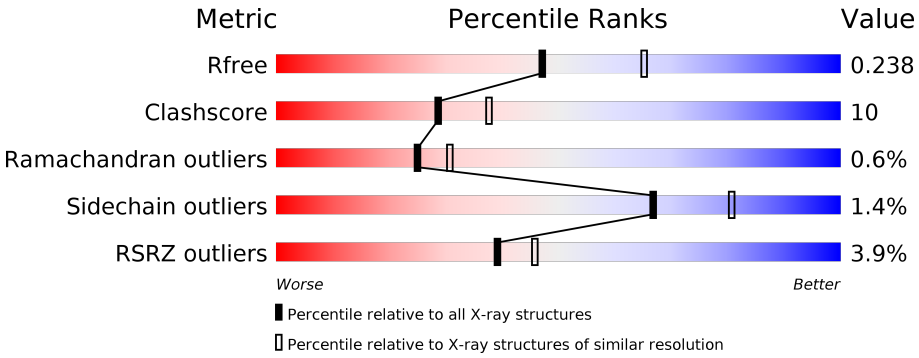
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	474	3% 83% 16%
1	B	474	5% 79% 18%

2 Entry composition

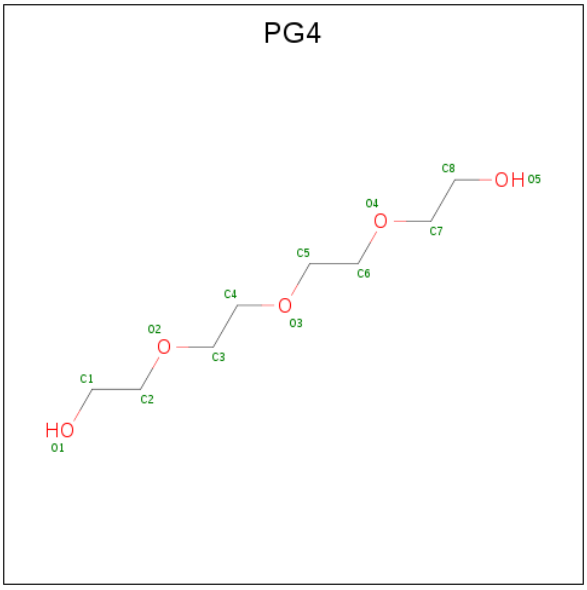
There are 4 unique types of molecules in this entry. The entry contains 14996 atoms, of which 7335 are hydrogens and 0 are deuteriums.

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 Thiol-activated cytolysin.

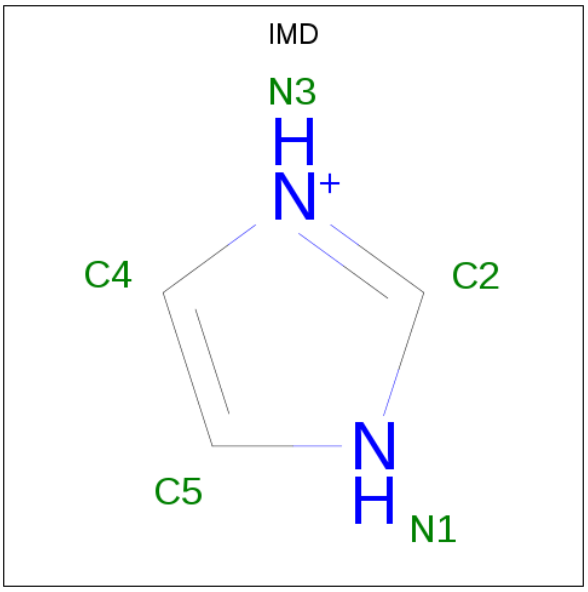
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	474	Total	C	H	N	O	S	Se	0	0	0
			7375	2358	3655	628	725	4	5			
1	B	473	Total	C	H	N	O	S	Se	0	0	0
			7368	2356	3652	627	724	4	5			

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N 10 3 5 2	0	0
3	B	1	Total C H N 10 3 5 2	0	0

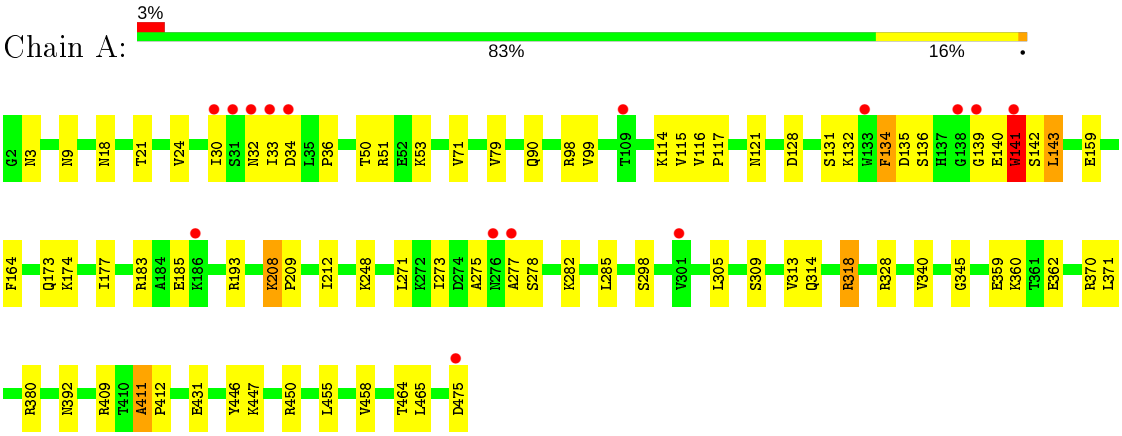
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	88	Total O 88 88	0	0
4	B	114	Total O 114 114	0	0

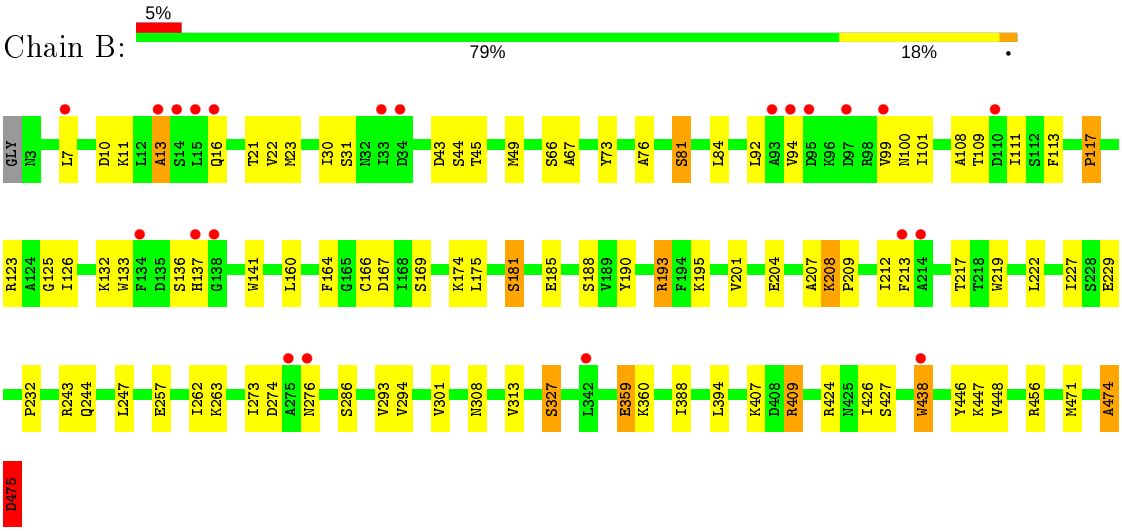
3 Residue-property plots (i)

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: Thiol-activated cytolysin



- Molecule 1: Thiol-activated cytolysin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.07Å 85.43Å 102.44Å 90.00° 101.05° 90.00°	Depositor
Resolution (Å)	43.45 – 2.30 44.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.45-2.30) 100.0 (44.98-2.20)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14_3247	Depositor
R, R_{free}	0.188 , 0.238 0.188 , 0.238	Depositor DCC
R_{free} test set	3011 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14996	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: PG4, IMD

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	0.72	2/3796 (0.1%)	0.82	4/5144 (0.1%)
1	B	0.78	7/3792 (0.2%)	0.93	9/5139 (0.2%)
All	All	0.75	9/7588 (0.1%)	0.88	13/10283 (0.1%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	475	ASP	CB-CG	12.95	1.78	1.51
1	A	141	TRP	CE3-CZ3	9.11	1.53	1.38
1	B	438	TRP	CZ3-CH2	-7.63	1.27	1.40
1	A	141	TRP	CZ3-CH2	-6.97	1.28	1.40
1	B	475	ASP	N-CA	6.05	1.58	1.46
1	B	359	GLU	CG-CD	5.83	1.60	1.51
1	B	257	GLU	CG-CD	5.75	1.60	1.51
1	B	294	VAL	CB-CG2	-5.14	1.42	1.52
1	B	475	ASP	CG-OD1	5.09	1.37	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	475	ASP	CB-CG-OD1	28.84	144.25	118.30
1	B	475	ASP	OD1-CG-OD2	-11.78	100.91	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	B	409	ARG	NE-CZ-NH1	-9.14	115.73	120.30
1	B	474	ALA	CA-C-N	7.65	134.03	117.20
1	A	318	ARG	NH1-CZ-NH2	7.39	127.53	119.40
1	B	456	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	474	ALA	CA-C-O	-6.15	107.18	120.10
1	B	193	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	474	ALA	CB-CA-C	-6.00	101.11	110.10
1	B	409	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	A	318	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	143	LEU	CB-CG-CD2	5.27	119.97	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TRP	Peptide
1	A	275	ALA	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	3720	3655	3655	65	3
1	B	3716	3652	3652	78	3
2	A	13	18	18	0	0
3	A	5	5	5	1	0
3	B	5	5	5	0	0
4	A	88	0	0	6	0
4	B	114	0	0	5	0
All	All	7661	7335	7335	143	3

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 10.

All (143) 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:475:ASP:CB	1:B:475:ASP:CG	1.79	1.52
1:B:49:MSE:HE2	1:B:359:GLU:HG3	1.34	1.08
1:B:407:LYS:HB2	1:B:409:ARG:NH1	1.78	0.98
1:B:167:ASP:OD1	4:B:601:HOH:O	1.84	0.93
1:B:49:MSE:HE2	1:B:359:GLU:CG	2.00	0.91
1:A:30:ILE:O	1:A:53:LYS:NZ	2.07	0.87
1:B:132:LYS:HE3	1:B:132:LYS:HA	1.57	0.85
1:A:273:ILE:HD11	1:A:285:LEU:HD13	1.58	0.85
1:B:101:ILE:HD11	1:B:113:PHE:CZ	2.12	0.85
1:B:407:LYS:HB2	1:B:409:ARG:HH12	1.40	0.84
1:B:101:ILE:HD11	1:B:113:PHE:CE2	2.13	0.84
1:A:135:ASP:OD2	1:A:328:ARG:NH2	2.12	0.83
1:B:11:LYS:HA	1:B:11:LYS:HE2	1.63	0.81
1:A:173:GLN:NE2	4:A:602:HOH:O	2.19	0.75
1:A:411:ALA:HB1	1:A:412:PRO:CD	2.18	0.74
1:A:134:PHE:HB2	1:A:140:GLU:HA	1.70	0.72
1:B:188:SER:OG	4:B:602:HOH:O	2.07	0.72
1:B:23:MSE:CE	1:B:84:LEU:HB3	2.25	0.67
1:B:94:VAL:HG11	1:B:222:LEU:HD23	1.75	0.67
1:A:411:ALA:HB1	1:A:412:PRO:HD2	1.75	0.67
1:B:447:LYS:HG3	1:B:471:MSE:CE	2.25	0.67
1:B:23:MSE:HE2	1:B:84:LEU:HB3	1.76	0.67
1:A:431:GLU:OE2	4:A:601:HOH:O	2.13	0.66
1:A:141:TRP:CG	1:A:142:SER:N	2.66	0.64
1:B:113:PHE:CE2	1:B:125:GLY:HA3	2.33	0.64
1:B:49:MSE:HE2	1:B:359:GLU:CD	2.18	0.63
1:A:18:ASN:OD1	1:A:21:THR:HG23	1.99	0.63
1:B:164:PHE:O	1:B:193:ARG:NH1	2.30	0.62
1:A:447:LYS:NZ	4:A:605:HOH:O	2.32	0.62
1:A:177:ILE:CD1	1:A:248:LYS:HD2	2.30	0.61
1:A:411:ALA:CB	1:A:412:PRO:CD	2.79	0.60
1:B:126:ILE:HD11	1:B:201:VAL:HG11	1.84	0.60
1:A:115:VAL:HG22	1:A:116:VAL:N	2.16	0.60
1:B:23:MSE:HE1	1:B:84:LEU:HD22	1.84	0.59
1:A:131:SER:O	1:A:135:ASP:HB2	2.04	0.58
1:A:411:ALA:CB	1:A:412:PRO:HD2	2.34	0.57
1:B:207:ALA:O	1:B:209:PRO:HD3	2.04	0.57
1:B:43:ASP:O	1:B:44:SER:HB2	2.05	0.57
1:A:177:ILE:HD11	1:A:248:LYS:HD2	1.87	0.56
1:A:380:ARG:NH2	4:A:601:HOH:O	2.37	0.56
1:A:273:ILE:HG22	1:A:313:VAL:HG11	1.88	0.56
1:B:113:PHE:CZ	1:B:125:GLY:HA3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ASP:O	1:B:13:ALA:HB2	2.06	0.55
1:B:175:LEU:HD21	1:B:293:VAL:HG23	1.89	0.54
1:B:94:VAL:HG11	1:B:222:LEU:CD2	2.37	0.54
1:B:209:PRO:O	1:B:212:ILE:HG22	2.06	0.54
1:A:464:THR:OG1	1:A:465:LEU:HD12	2.08	0.54
1:A:140:GLU:OE2	1:A:328:ARG:N	2.34	0.54
1:A:273:ILE:HD11	1:A:285:LEU:CD1	2.35	0.54
1:A:32:ASN:HB2	1:A:34:ASP:OD1	2.08	0.53
1:B:174:LYS:HD2	1:B:301:VAL:HG21	1.91	0.53
1:A:282:LYS:HA	1:A:285:LEU:HD12	1.91	0.52
1:B:273:ILE:HD12	1:B:313:VAL:CG2	2.38	0.52
1:A:371:LEU:HD23	1:A:458:VAL:HG22	1.91	0.52
1:A:164:PHE:O	1:A:193:ARG:NH1	2.42	0.52
1:B:407:LYS:HB2	1:B:409:ARG:HH11	1.70	0.52
1:A:142:SER:O	1:A:143:LEU:HD23	2.11	0.51
1:B:108:ALA:HB2	1:B:133:TRP:CZ3	2.44	0.51
1:A:36:PRO:HD2	1:A:51:ARG:NH2	2.25	0.51
1:B:175:LEU:HG	1:B:293:VAL:HG21	1.91	0.51
1:A:273:ILE:O	1:A:273:ILE:HG23	2.10	0.51
1:B:99:VAL:HG23	1:B:101:ILE:HG23	1.93	0.51
1:B:447:LYS:HG3	1:B:471:MSE:HE1	1.92	0.51
1:A:9:ASN:ND2	1:A:208:LYS:HD2	2.25	0.50
1:A:309:SER:O	1:A:313:VAL:HG23	2.12	0.50
1:B:273:ILE:HD12	1:B:313:VAL:HG21	1.94	0.50
1:B:30:ILE:HG22	1:B:31:SER:O	2.12	0.50
1:A:173:GLN:OE1	1:A:174:LYS:HE2	2.12	0.49
1:A:159:GLU:OE1	3:A:502:IMD:H4	2.12	0.49
1:A:314:GLN:HG2	1:A:318:ARG:HH21	1.77	0.49
1:B:243:ARG:HG2	1:B:244:GLN:N	2.28	0.49
1:A:3:ASN:OD1	1:A:3:ASN:N	2.46	0.48
1:B:66:SER:O	1:B:67:ALA:HB3	2.12	0.48
1:A:139:GLY:C	1:A:140:GLU:HG2	2.34	0.48
1:B:247:LEU:N	1:B:247:LEU:HD12	2.29	0.48
1:B:274:ASP:HB2	1:B:276:ASN:OD1	2.14	0.48
1:A:340:VAL:HG22	1:A:345:GLY:C	2.35	0.47
1:B:92:LEU:HD12	1:B:227:ILE:HD11	1.96	0.47
1:B:49:MSE:CE	1:B:359:GLU:CD	2.82	0.47
1:B:11:LYS:HA	1:B:11:LYS:CE	2.33	0.47
1:A:392:ASN:HB2	4:A:629:HOH:O	2.14	0.47
1:B:11:LYS:HG3	1:B:219:TRP:CD2	2.50	0.47
1:A:271:LEU:HD12	1:A:271:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG22	1:A:90:GLN:HB3	1.96	0.46
1:B:16:GLN:O	1:B:229:GLU:HB3	2.16	0.46
1:A:139:GLY:O	1:A:140:GLU:HG2	2.15	0.46
1:B:23:MSE:CE	1:B:84:LEU:CB	2.93	0.46
1:A:277:ALA:O	1:A:278:SER:OG	2.24	0.46
1:B:175:LEU:CD2	1:B:293:VAL:HG23	2.46	0.46
1:A:305:LEU:HD12	1:A:305:LEU:N	2.31	0.45
1:B:181:SER:O	1:B:185:GLU:HG3	2.16	0.45
1:A:177:ILE:HD13	1:A:248:LYS:HD2	1.97	0.45
1:B:388:ILE:HD13	1:B:424:ARG:HD3	1.99	0.45
1:A:115:VAL:HG21	1:A:121:ASN:HB3	1.98	0.45
1:B:360:LYS:HE2	1:B:360:LYS:O	2.17	0.45
1:A:128:ASP:OD2	1:A:132:LYS:HE3	2.17	0.44
1:B:73:TYR:CE1	1:B:76:ALA:HB2	2.53	0.44
1:A:273:ILE:CD1	1:A:285:LEU:HD13	2.38	0.44
1:A:305:LEU:N	1:A:305:LEU:CD1	2.81	0.44
1:B:99:VAL:CG2	1:B:117:PRO:HG3	2.47	0.44
1:B:22:VAL:HG21	1:B:232:PRO:HD2	2.00	0.44
1:B:141:TRP:CD1	1:B:327:SER:HB2	2.51	0.44
1:B:394:LEU:HA	1:B:394:LEU:HD23	1.85	0.44
1:A:360:LYS:NZ	1:A:362:GLU:OE1	2.47	0.44
1:B:447:LYS:HG3	1:B:471:MSE:HE3	1.98	0.44
1:A:24:VAL:HG13	1:A:24:VAL:O	2.17	0.44
1:A:71:VAL:O	1:A:71:VAL:CG1	2.65	0.44
1:A:99:VAL:HB	1:A:117:PRO:HG3	2.00	0.43
1:B:474:ALA:O	1:B:475:ASP:CB	2.65	0.43
1:B:21:THR:HG22	1:B:21:THR:O	2.18	0.43
1:B:7:LEU:O	1:B:7:LEU:HD12	2.18	0.43
1:B:109:THR:HG23	1:B:111:ILE:HG13	2.01	0.43
1:B:475:ASP:OD2	1:B:475:ASP:CB	2.53	0.43
1:A:115:VAL:CG2	1:A:116:VAL:N	2.81	0.43
1:B:43:ASP:O	1:B:44:SER:CB	2.66	0.43
1:B:100:ASN:HB3	1:B:204:GLU:CD	2.40	0.42
1:B:407:LYS:CB	1:B:409:ARG:NH1	2.66	0.42
1:A:99:VAL:CG2	1:A:212:ILE:HD12	2.49	0.42
1:B:427:SER:HB2	1:B:448:VAL:HG12	2.00	0.42
1:A:33:ILE:O	1:A:33:ILE:HG13	2.18	0.42
1:A:51:ARG:HG2	1:A:359:GLU:HG2	2.00	0.42
1:A:98:ARG:NH2	1:A:114:LYS:HD3	2.34	0.42
1:B:213:PHE:HB3	1:B:217:THR:OG1	2.20	0.42
1:A:209:PRO:O	1:A:212:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:SER:HA	1:B:308:ASN:OD1	2.19	0.42
1:A:450:ARG:HE	1:A:475:ASP:HB2	1.84	0.42
1:B:23:MSE:HE3	1:B:81:SER:H	1.85	0.42
1:B:160:LEU:HD22	1:B:166:CYS:SG	2.61	0.41
1:B:190:TYR:CD2	1:B:262:ILE:HG21	2.55	0.41
1:A:116:VAL:O	1:A:116:VAL:HG23	2.20	0.41
1:A:370:ARG:HG3	1:A:455:LEU:HD11	2.02	0.41
1:B:175:LEU:HG	1:B:293:VAL:CG2	2.51	0.41
1:B:195:LYS:NZ	4:B:617:HOH:O	2.53	0.41
1:A:183:ARG:O	1:A:185:GLU:O	2.38	0.41
1:A:248:LYS:NZ	4:A:623:HOH:O	2.54	0.41
1:B:123:ARG:HG3	4:B:636:HOH:O	2.21	0.41
1:B:169:SER:HB3	4:B:601:HOH:O	2.19	0.41
1:B:43:ASP:C	1:B:45:THR:H	2.23	0.41
1:B:66:SER:O	1:B:67:ALA:CB	2.68	0.41
1:A:50:THR:CG2	1:A:360:LYS:HB3	2.51	0.40
1:B:136:SER:O	1:B:137:HIS:ND1	2.54	0.40
1:A:134:PHE:O	1:A:139:GLY:O	2.39	0.40
1:B:426:ILE:N	1:B:426:ILE:HD12	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TRP:CZ3	1:B:438:TRP:HE3[3_445]	1.27	0.33
1:A:141:TRP:HZ3	1:B:438:TRP:HE3[3_445]	1.33	0.27
1:A:141:TRP:CZ3	1:B:438:TRP:CE3[3_445]	2.01	0.19

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	472/474 (100%)	445 (94%)	25 (5%)	2 (0%)	34 42
1	B	471/474 (99%)	448 (95%)	19 (4%)	4 (1%)	19 23
All	All	943/948 (100%)	893 (95%)	44 (5%)	6 (1%)	25 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	SER
1	A	411	ALA
1	B	81	SER
1	B	13	ALA
1	B	208	LYS
1	B	117	PRO

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	406/401 (101%)	401 (99%)	5 (1%)	71 84
1	B	406/401 (101%)	400 (98%)	6 (2%)	65 79
All	All	812/802 (101%)	801 (99%)	11 (1%)	67 81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	PHE
1	A	136	SER
1	A	208	LYS
1	A	409	ARG
1	A	446	TYR
1	B	181	SER
1	B	208	LYS
1	B	263	LYS
1	B	327	SER
1	B	446	TYR

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Mol	Chain	Res	Type
1	B	475	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	240	GLN
1	A	287	GLN
1	B	173	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

3 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	$\#\|Z\| > 2$
3	IMD	A	502	-	3,5,5	0.50	0	4,5,5	0.74	0
3	IMD	B	501	-	3,5,5	0.54	0	4,5,5	0.52	0
2	PG4	A	501	-	12,12,12	0.59	0	11,11,11	0.68	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
3	IMD	A	502	-	-	-	0/1/1/1
3	IMD	B	501	-	-	-	0/1/1/1
2	PG4	A	501	-	-	8/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PG4	O1-C1-C2-O2
2	A	501	PG4	O2-C3-C4-O3
2	A	501	PG4	C5-C6-O4-C7
2	A	501	PG4	C4-C3-O2-C2
2	A	501	PG4	C6-C5-O3-C4
2	A	501	PG4	C3-C4-O3-C5
2	A	501	PG4	O4-C7-C8-O5
2	A	501	PG4	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	IMD	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	469/474 (98%)	0.24	15 (3%) 47 54	30, 50, 83, 123	0
1	B	468/474 (98%)	0.32	22 (4%) 31 38	29, 50, 85, 116	0
All	All	937/948 (98%)	0.28	37 (3%) 39 46	29, 50, 85, 123	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ILE	8.4
1	A	141	TRP	7.5
1	B	14	SER	7.0
1	A	276	ASN	4.9
1	B	33	ILE	4.5
1	B	275	ALA	4.0
1	A	277	ALA	3.9
1	A	31	SER	3.8
1	B	34	ASP	3.6
1	B	438	TRP	3.5
1	B	214	ALA	3.5
1	A	186	LYS	3.4
1	B	93	ALA	3.1
1	B	16	GLN	3.0
1	B	15	LEU	2.9
1	B	95	ASP	2.9
1	B	97	ASP	2.8
1	A	475	ASP	2.8
1	A	109	THR	2.8
1	A	32	ASN	2.6
1	B	342	LEU	2.6
1	B	134	PHE	2.5
1	B	110	ASP	2.5
1	A	34	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	94	VAL	2.4
1	B	138	GLY	2.4
1	A	133	TRP	2.4
1	A	301	VAL	2.4
1	B	99	VAL	2.3
1	B	276	ASN	2.2
1	A	139	GLY	2.2
1	B	13	ALA	2.2
1	B	7	LEU	2.1
1	B	213	PHE	2.1
1	A	30	ILE	2.1
1	A	138	GLY	2.0
1	B	137	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	IMD	B	501	5/5	0.87	0.18	42,51,59,71	0
3	IMD	A	502	5/5	0.89	0.19	38,61,74,75	0
2	PG4	A	501	13/13	0.91	0.15	48,61,74,78	0

6.5 Other polymers (i)

There are no such residues in this entry.