Full wwPDB X-ray Structure Validation Report

Jun 16, 2024 – 04:19 AM EDT

PDB ID	:	2PMB
Title	:	Crystal structure of predicted nucleotide-binding protein from Vibrio cholerae
Authors	:	Patskovsky, Y.; Zhan, C.; Shi, W.; Toro, R.; Sauder, J.M.; Gilmore, J.; Iizuka, M.; Maletic, M.; Gheyi, T.; Wasserman, S.R.; Smith, D.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-04-20
Resolution	:	1.99 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 (1)) were used in the production of this report:

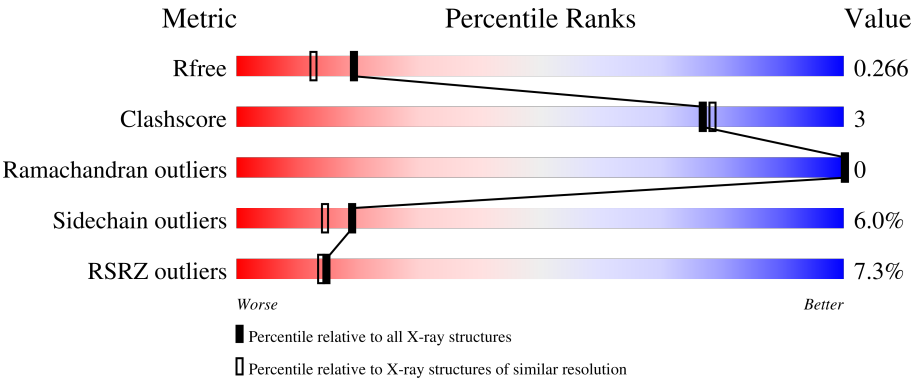
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	462	8% 83% 11% 5%
1	B	462	7% 84% 9% • 5%
1	C	462	6% 84% 10% • 6%
1	D	462	6% 81% 12% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14539 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	Se	0	9	0
			3483	2214	606	640	5	18			
1	B	437	Total	C	N	O	S	Se	0	8	0
			3479	2210	605	641	5	18			
1	C	434	Total	C	N	O	S	Se	0	12	0
			3484	2217	609	634	5	19			
1	D	437	Total	C	N	O	S	Se	0	8	0
			3478	2210	607	638	5	18			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MSE	-	cloning artifact	UNP Q9KTK3
A	5	SER	-	cloning artifact	UNP Q9KTK3
A	6	LEU	-	cloning artifact	UNP Q9KTK3
A	16	MSE	MET	modified residue	UNP Q9KTK3
A	71	MSE	MET	modified residue	UNP Q9KTK3
A	114	MSE	MET	modified residue	UNP Q9KTK3
A	192	MSE	MET	modified residue	UNP Q9KTK3
A	196	MSE	MET	modified residue	UNP Q9KTK3
A	237	MSE	MET	modified residue	UNP Q9KTK3
A	250	MSE	MET	modified residue	UNP Q9KTK3
A	274	MSE	MET	modified residue	UNP Q9KTK3
A	275	MSE	MET	modified residue	UNP Q9KTK3
A	284	MSE	MET	modified residue	UNP Q9KTK3
A	331	MSE	MET	modified residue	UNP Q9KTK3
A	335	MSE	MET	modified residue	UNP Q9KTK3
A	372	MSE	MET	modified residue	UNP Q9KTK3
A	418	MSE	MET	modified residue	UNP Q9KTK3
A	425	MSE	MET	modified residue	UNP Q9KTK3
A	428	MSE	MET	modified residue	UNP Q9KTK3
A	441	MSE	MET	modified residue	UNP Q9KTK3
A	458	GLU	-	cloning artifact	UNP Q9KTK3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	459	GLY	-	cloning artifact	UNP Q9KTK3
A	460	HIS	-	cloning artifact	UNP Q9KTK3
A	461	HIS	-	cloning artifact	UNP Q9KTK3
A	462	HIS	-	cloning artifact	UNP Q9KTK3
A	463	HIS	-	cloning artifact	UNP Q9KTK3
A	464	HIS	-	cloning artifact	UNP Q9KTK3
A	465	HIS	-	cloning artifact	UNP Q9KTK3
B	4	MSE	-	cloning artifact	UNP Q9KTK3
B	5	SER	-	cloning artifact	UNP Q9KTK3
B	6	LEU	-	cloning artifact	UNP Q9KTK3
B	16	MSE	MET	modified residue	UNP Q9KTK3
B	71	MSE	MET	modified residue	UNP Q9KTK3
B	114	MSE	MET	modified residue	UNP Q9KTK3
B	192	MSE	MET	modified residue	UNP Q9KTK3
B	196	MSE	MET	modified residue	UNP Q9KTK3
B	237	MSE	MET	modified residue	UNP Q9KTK3
B	250	MSE	MET	modified residue	UNP Q9KTK3
B	274	MSE	MET	modified residue	UNP Q9KTK3
B	275	MSE	MET	modified residue	UNP Q9KTK3
B	284	MSE	MET	modified residue	UNP Q9KTK3
B	331	MSE	MET	modified residue	UNP Q9KTK3
B	335	MSE	MET	modified residue	UNP Q9KTK3
B	372	MSE	MET	modified residue	UNP Q9KTK3
B	418	MSE	MET	modified residue	UNP Q9KTK3
B	425	MSE	MET	modified residue	UNP Q9KTK3
B	428	MSE	MET	modified residue	UNP Q9KTK3
B	441	MSE	MET	modified residue	UNP Q9KTK3
B	458	GLU	-	cloning artifact	UNP Q9KTK3
B	459	GLY	-	cloning artifact	UNP Q9KTK3
B	460	HIS	-	cloning artifact	UNP Q9KTK3
B	461	HIS	-	cloning artifact	UNP Q9KTK3
B	462	HIS	-	cloning artifact	UNP Q9KTK3
B	463	HIS	-	cloning artifact	UNP Q9KTK3
B	464	HIS	-	cloning artifact	UNP Q9KTK3
B	465	HIS	-	cloning artifact	UNP Q9KTK3
C	4	MSE	-	cloning artifact	UNP Q9KTK3
C	5	SER	-	cloning artifact	UNP Q9KTK3
C	6	LEU	-	cloning artifact	UNP Q9KTK3
C	16	MSE	MET	modified residue	UNP Q9KTK3
C	71	MSE	MET	modified residue	UNP Q9KTK3
C	114	MSE	MET	modified residue	UNP Q9KTK3
C	192	MSE	MET	modified residue	UNP Q9KTK3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	196	MSE	MET	modified residue	UNP Q9KTK3
C	237	MSE	MET	modified residue	UNP Q9KTK3
C	250	MSE	MET	modified residue	UNP Q9KTK3
C	274	MSE	MET	modified residue	UNP Q9KTK3
C	275	MSE	MET	modified residue	UNP Q9KTK3
C	284	MSE	MET	modified residue	UNP Q9KTK3
C	331	MSE	MET	modified residue	UNP Q9KTK3
C	335	MSE	MET	modified residue	UNP Q9KTK3
C	372	MSE	MET	modified residue	UNP Q9KTK3
C	418	MSE	MET	modified residue	UNP Q9KTK3
C	425	MSE	MET	modified residue	UNP Q9KTK3
C	428	MSE	MET	modified residue	UNP Q9KTK3
C	441	MSE	MET	modified residue	UNP Q9KTK3
C	458	GLU	-	cloning artifact	UNP Q9KTK3
C	459	GLY	-	cloning artifact	UNP Q9KTK3
C	460	HIS	-	cloning artifact	UNP Q9KTK3
C	461	HIS	-	cloning artifact	UNP Q9KTK3
C	462	HIS	-	cloning artifact	UNP Q9KTK3
C	463	HIS	-	cloning artifact	UNP Q9KTK3
C	464	HIS	-	cloning artifact	UNP Q9KTK3
C	465	HIS	-	cloning artifact	UNP Q9KTK3
D	4	MSE	-	cloning artifact	UNP Q9KTK3
D	5	SER	-	cloning artifact	UNP Q9KTK3
D	6	LEU	-	cloning artifact	UNP Q9KTK3
D	16	MSE	MET	modified residue	UNP Q9KTK3
D	71	MSE	MET	modified residue	UNP Q9KTK3
D	114	MSE	MET	modified residue	UNP Q9KTK3
D	192	MSE	MET	modified residue	UNP Q9KTK3
D	196	MSE	MET	modified residue	UNP Q9KTK3
D	237	MSE	MET	modified residue	UNP Q9KTK3
D	250	MSE	MET	modified residue	UNP Q9KTK3
D	274	MSE	MET	modified residue	UNP Q9KTK3
D	275	MSE	MET	modified residue	UNP Q9KTK3
D	284	MSE	MET	modified residue	UNP Q9KTK3
D	331	MSE	MET	modified residue	UNP Q9KTK3
D	335	MSE	MET	modified residue	UNP Q9KTK3
D	372	MSE	MET	modified residue	UNP Q9KTK3
D	418	MSE	MET	modified residue	UNP Q9KTK3
D	425	MSE	MET	modified residue	UNP Q9KTK3
D	428	MSE	MET	modified residue	UNP Q9KTK3
D	441	MSE	MET	modified residue	UNP Q9KTK3
D	458	GLU	-	cloning artifact	UNP Q9KTK3

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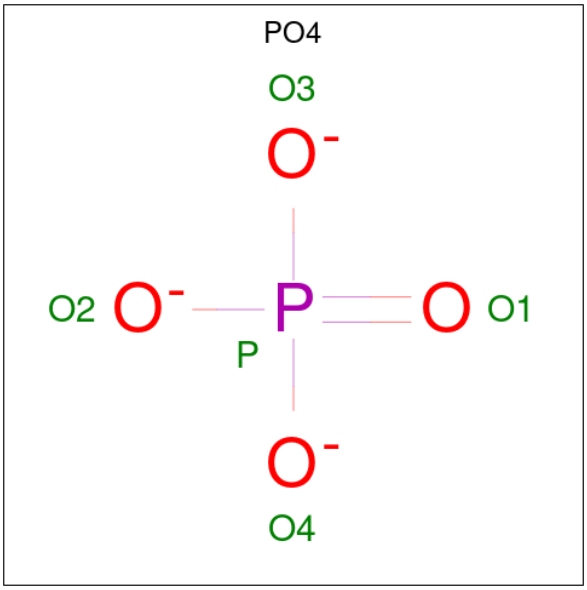
Chain	Residue	Modelled	Actual	Comment	Reference
D	459	GLY	-	cloning artifact	UNP Q9KTK3
D	460	HIS	-	cloning artifact	UNP Q9KTK3
D	461	HIS	-	cloning artifact	UNP Q9KTK3
D	462	HIS	-	cloning artifact	UNP Q9KTK3
D	463	HIS	-	cloning artifact	UNP Q9KTK3
D	464	HIS	-	cloning artifact	UNP Q9KTK3
D	465	HIS	-	cloning artifact	UNP Q9KTK3

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0

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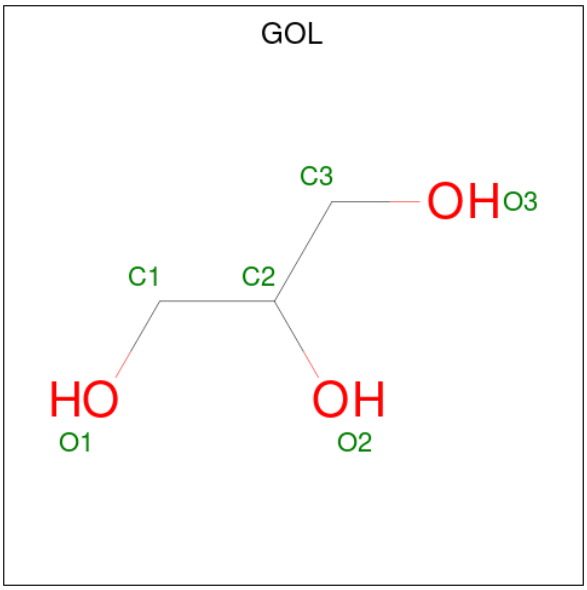
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	138	Total O 138 138	0	0
4	B	149	Total O 149 149	0	0
4	C	124	Total O 124 124	0	0

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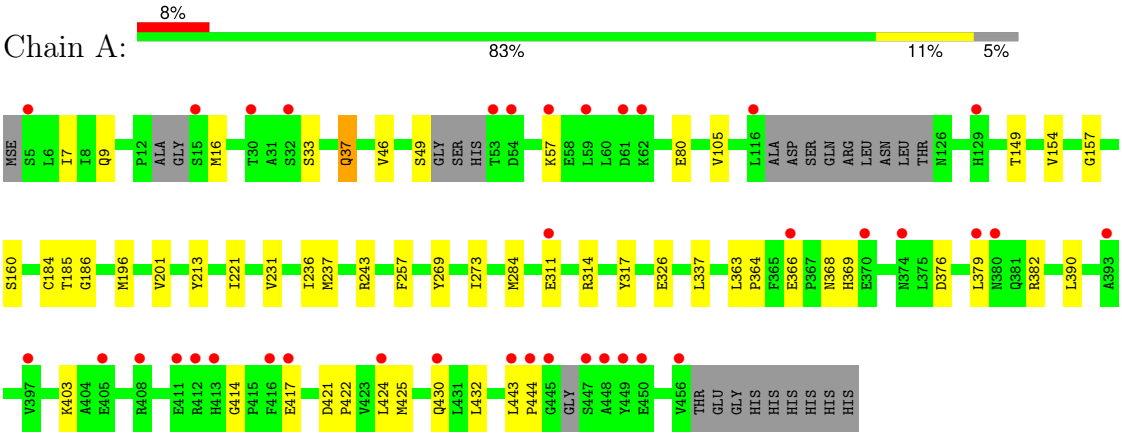
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	132	Total 132	O 132	0	0

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.

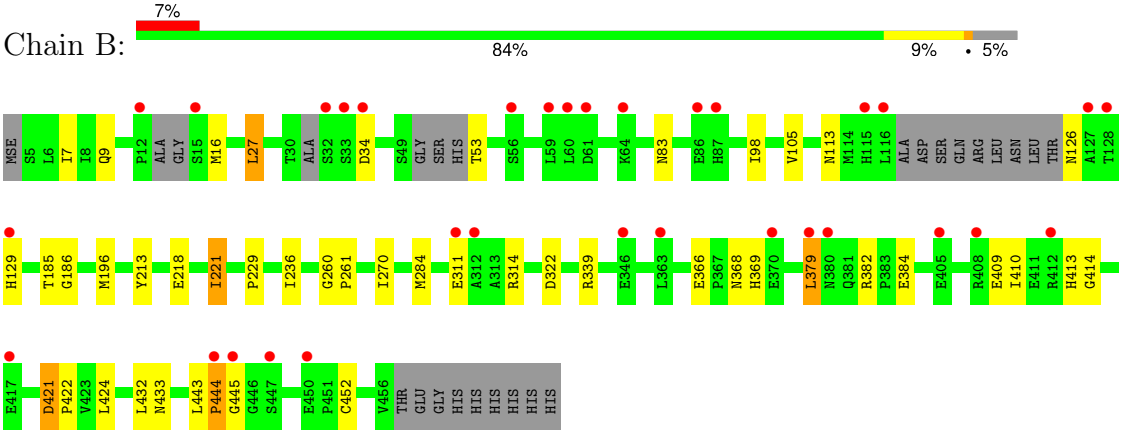
• Molecule 1: Uncharacterized protein

Chain A:



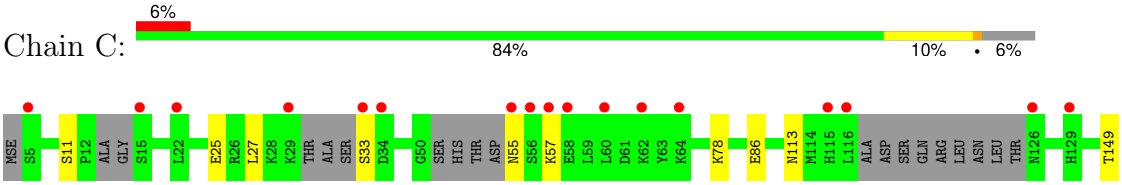
• Molecule 1: Uncharacterized protein

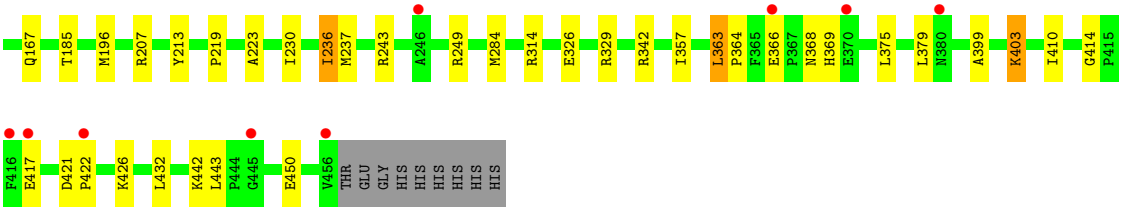
Chain B:



• Molecule 1: Uncharacterized protein

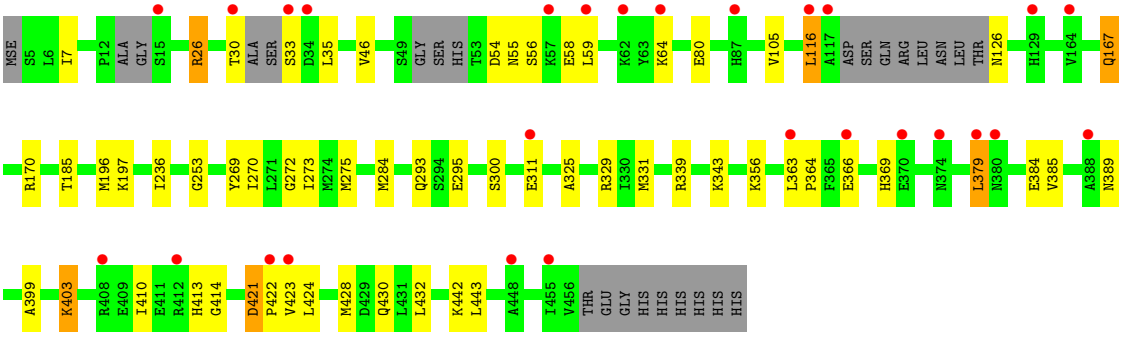
Chain C:





• Molecule 1: Uncharacterized protein

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	58.80Å 178.22Å 89.51Å 90.00° 103.78° 90.00°	Depositor
Resolution (Å)	20.00 – 1.99 19.70 – 1.99	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-1.99) 90.5 (19.70-1.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.208 , 0.266 0.208 , 0.266	Depositor DCC
R_{free} test set	3331 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14539	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: GOL, PO4

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	0.43	0/3562	0.58	0/4787
1	B	0.41	0/3556	0.57	1/4777 (0.0%)
1	C	0.42	0/3573	0.59	0/4797
1	D	0.41	0/3555	0.58	1/4775 (0.0%)
All	All	0.42	0/14246	0.58	2/19136 (0.0%)

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	B	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	27	LEU	CA-CB-CG	7.17	131.79	115.30
1	D	116	LEU	CA-CB-CG	6.14	129.42	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	444	PRO	Peptide
1	B	445	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	D	58	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3483	0	3514	22	0
1	B	3479	0	3501	16	0
1	C	3484	0	3520	21	0
1	D	3478	0	3507	28	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	1	0
3	B	6	0	8	0	0
3	C	6	0	8	3	0
4	A	138	0	0	1	0
4	B	149	0	0	0	0
4	C	124	0	0	1	0
4	D	132	0	0	1	0
All	All	14539	0	14058	85	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 3.

All (85) 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:167[A]:GLN:HG3	1:D:170[A]:ARG:HH22	1.38	0.86
1:C:249:ARG:HH22	3:C:701:GOL:H11	1.49	0.78
1:D:167[A]:GLN:HG3	1:D:170[A]:ARG:NH2	2.07	0.70
1:C:357:ILE:H	3:C:701:GOL:H12	1.57	0.68
1:C:185:THR:HG22	1:C:196:MSE:HE3	1.75	0.68
1:A:369:HIS:CE1	1:A:414:GLY:O	2.48	0.67
1:D:167[A]:GLN:OE1	1:D:170[A]:ARG:NH2	2.33	0.61
1:D:185:THR:HG22	1:D:196:MSE:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:HIS:HE1	1:A:414:GLY:O	1.85	0.59
1:D:30:THR:HG1	1:D:33:SER:N	2.03	0.57
1:C:219:PRO:HG3	1:C:236:ILE:HD11	1.87	0.56
1:C:399:ALA:HA	1:C:403:LYS:HD3	1.87	0.56
1:B:369:HIS:NE2	1:B:414:GLY:O	2.25	0.55
1:A:105:VAL:HA	1:A:236:ILE:HD13	1.89	0.54
1:C:369:HIS:NE2	1:C:414:GLY:O	2.39	0.54
1:D:369:HIS:NE2	1:D:414:GLY:O	2.38	0.53
1:B:185:THR:HG23	1:B:186:GLY:O	2.10	0.52
1:B:369:HIS:CE1	1:B:413:HIS:HB2	2.45	0.51
1:C:237:MSE:HG3	1:C:243:ARG:HA	1.91	0.51
1:B:379:LEU:HD12	1:B:424:LEU:HB2	1.93	0.51
1:D:339:ARG:HD3	4:D:691:HOH:O	2.11	0.51
1:A:237:MSE:HG3	1:A:243:ARG:HA	1.93	0.51
1:B:369:HIS:HE1	1:B:409:GLU:O	1.93	0.50
1:B:410:ILE:HD13	1:B:452:CYS:HB2	1.92	0.50
1:A:37:GLN:NE2	4:A:748:HOH:O	2.45	0.50
1:A:185:THR:HG22	1:A:196:MSE:HE3	1.93	0.50
1:A:185:THR:HG23	1:A:186:GLY:O	2.11	0.50
1:B:270:ILE:HD11	1:B:284[A]:MSE:HE1	1.94	0.50
1:D:167[A]:GLN:CG	1:D:170[A]:ARG:HH22	2.18	0.49
1:B:105:VAL:HA	1:B:236:ILE:HD13	1.94	0.48
1:A:390:LEU:HD21	1:A:424:LEU:HD11	1.95	0.48
1:C:326:GLU:HA	1:C:329[B]:ARG:HG2	1.95	0.48
1:D:197:LYS:NZ	2:D:602:PO4:O2	2.43	0.47
1:A:269:TYR:O	1:A:273[A]:ILE:HG12	2.14	0.47
1:A:284[A]:MSE:HE2	1:A:284[A]:MSE:HB3	1.85	0.47
1:C:249:ARG:NH2	3:C:701:GOL:H11	2.24	0.47
1:C:57:LYS:HG2	1:C:223:ALA:HB3	1.96	0.47
1:D:55:ASN:ND2	1:D:443:LEU:H	2.13	0.47
1:A:201:VAL:HG13	1:C:230:ILE:HD12	1.97	0.47
1:D:55:ASN:HD21	1:D:442[A]:LYS:HA	1.80	0.46
1:C:369:HIS:CE1	1:C:414:GLY:O	2.69	0.46
1:D:325:ALA:O	1:D:329:ARG:HB2	2.16	0.46
1:C:55:ASN:HD21	1:C:442:LYS:HA	1.80	0.46
1:B:126:ASN:OD1	1:B:129:HIS:ND1	2.48	0.45
1:A:424:LEU:HG	1:A:425:MSE:HE2	1.98	0.45
1:D:55:ASN:HD21	1:D:442[B]:LYS:HA	1.80	0.45
1:D:55:ASN:HD21	1:D:443:LEU:H	1.64	0.45
1:D:7:ILE:HG23	1:D:80:GLU:HG3	1.97	0.45
1:D:269:TYR:O	1:D:273:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113[B]:ASN:ND2	4:C:789:HOH:O	2.49	0.45
1:C:284[B]:MSE:CE	1:C:342:ARG:HH21	2.30	0.45
1:B:196:MSE:SE	1:B:213:TYR:HB3	2.67	0.45
1:C:284[B]:MSE:HE2	1:C:342:ARG:HH21	1.82	0.45
1:A:154:VAL:HA	1:A:184:CYS:O	2.17	0.44
1:B:421:ASP:HA	1:B:422:PRO:HD3	1.86	0.44
1:D:253:GLY:HA3	1:D:331:MSE:SE	2.68	0.44
1:B:98:ILE:HG13	1:B:229:PRO:HB3	2.00	0.44
1:D:105:VAL:HA	1:D:236:ILE:HD13	2.00	0.43
1:A:422:PRO:HA	1:A:425:MSE:HB2	2.00	0.43
1:A:196:MSE:HE2	1:A:213:TYR:HB3	2.00	0.43
1:D:379:LEU:HD12	1:D:424:LEU:HB2	2.01	0.43
1:A:231:VAL:O	1:C:207:ARG:NH2	2.52	0.43
1:C:196:MSE:HE2	1:C:213:TYR:HB3	2.01	0.43
1:D:369:HIS:CE1	1:D:413:HIS:HB2	2.53	0.43
1:B:260:GLY:HA3	1:B:261:PRO:HD2	1.84	0.43
1:D:284[B]:MSE:HE2	1:D:284[B]:MSE:HB2	1.96	0.43
1:A:9:GLN:HG2	1:A:80:GLU:HG3	2.01	0.42
1:A:363:LEU:HA	1:A:364:PRO:HD3	1.89	0.42
1:A:314[B]:ARG:NH1	1:A:317:TYR:O	2.52	0.42
1:D:385:VAL:O	1:D:389:ASN:ND2	2.52	0.42
1:A:443:LEU:HA	1:A:444:PRO:HD3	1.78	0.42
1:C:363:LEU:HA	1:C:364:PRO:HD3	1.87	0.42
1:D:270:ILE:HD11	1:D:284[A]:MSE:HE1	2.00	0.42
1:D:26:ARG:HB2	1:D:35:LEU:HD23	2.02	0.42
1:D:399:ALA:HA	1:D:403:LYS:HB2	2.01	0.42
1:D:363:LEU:HA	1:D:364:PRO:HD3	1.91	0.41
1:A:157:GLY:HA3	1:A:257:PHE:HB2	2.02	0.41
1:B:443:LEU:HA	1:B:444:PRO:HD3	1.92	0.41
1:B:185:THR:HG22	1:B:196:MSE:HE3	2.03	0.41
1:C:421:ASP:HA	1:C:422:PRO:HD3	1.85	0.41
1:C:55:ASN:HB3	1:C:443:LEU:HD12	2.02	0.41
1:A:57:LYS:HE2	1:A:57:LYS:HB3	1.92	0.40
1:B:218:GLU:HG3	1:B:221:ILE:HG22	2.03	0.40
1:D:421:ASP:HA	1:D:422:PRO:HD3	1.84	0.40
1:D:272:GLY:HA2	1:D:275:MSE:HE2	2.03	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	436/462 (94%)	423 (97%)	13 (3%)	0	100	100
1	B	435/462 (94%)	419 (96%)	16 (4%)	0	100	100
1	C	436/462 (94%)	424 (97%)	12 (3%)	0	100	100
1	D	434/462 (94%)	426 (98%)	8 (2%)	0	100	100
All	All	1741/1848 (94%)	1692 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	381/373 (102%)	357 (94%)	24 (6%)	18	13
1	B	380/373 (102%)	356 (94%)	24 (6%)	18	13
1	C	380/373 (102%)	357 (94%)	23 (6%)	18	14
1	D	379/373 (102%)	352 (93%)	27 (7%)	14	10
All	All	1520/1492 (102%)	1422 (94%)	98 (6%)	19	13

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	16	MSE

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Mol	Chain	Res	Type
1	A	33	SER
1	A	37	GLN
1	A	46	VAL
1	A	49	SER
1	A	149[A]	THR
1	A	149[B]	THR
1	A	160	SER
1	A	221	ILE
1	A	311	GLU
1	A	326	GLU
1	A	337	LEU
1	A	366[A]	GLU
1	A	366[B]	GLU
1	A	368	ASN
1	A	376	ASP
1	A	379	LEU
1	A	382	ARG
1	A	403	LYS
1	A	417	GLU
1	A	421	ASP
1	A	430	GLN
1	A	432	LEU
1	B	7	ILE
1	B	9	GLN
1	B	16	MSE
1	B	27	LEU
1	B	34	ASP
1	B	53	THR
1	B	83	ASN
1	B	113[A]	ASN
1	B	113[B]	ASN
1	B	221	ILE
1	B	311[A]	GLU
1	B	311[B]	GLU
1	B	314	ARG
1	B	322	ASP
1	B	339	ARG
1	B	366[A]	GLU
1	B	366[B]	GLU
1	B	368	ASN
1	B	379	LEU
1	B	382	ARG

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Mol	Chain	Res	Type
1	B	384	GLU
1	B	421	ASP
1	B	432	LEU
1	B	433	ASN
1	C	11	SER
1	C	25[A]	GLU
1	C	25[B]	GLU
1	C	27	LEU
1	C	33	SER
1	C	78	LYS
1	C	86	GLU
1	C	149	THR
1	C	167	GLN
1	C	236	ILE
1	C	314	ARG
1	C	363	LEU
1	C	366[A]	GLU
1	C	366[B]	GLU
1	C	368	ASN
1	C	375	LEU
1	C	379	LEU
1	C	403	LYS
1	C	410	ILE
1	C	417	GLU
1	C	426	LYS
1	C	432	LEU
1	C	450	GLU
1	D	26	ARG
1	D	46	VAL
1	D	54	ASP
1	D	56	SER
1	D	59	LEU
1	D	64	LYS
1	D	116	LEU
1	D	126	ASN
1	D	167[A]	GLN
1	D	167[B]	GLN
1	D	293	GLN
1	D	295	GLU
1	D	300	SER
1	D	311	GLU
1	D	343	LYS

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Mol	Chain	Res	Type
1	D	356	LYS
1	D	366[A]	GLU
1	D	366[B]	GLU
1	D	379	LEU
1	D	384	GLU
1	D	403	LYS
1	D	410	ILE
1	D	421	ASP
1	D	423	VAL
1	D	428	MSE
1	D	430	GLN
1	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	368	ASN
1	A	369	HIS
1	A	378	HIS
1	A	433	ASN
1	B	368	ASN
1	B	433	ASN
1	C	55	ASN
1	C	115	HIS
1	C	126	ASN
1	C	368	ASN
1	C	381	GLN
1	C	389	ASN
1	D	37	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	D	601	-	4,4,4	1.09	0	6,6,6	0.32	0
2	PO4	B	607	-	4,4,4	0.77	0	6,6,6	0.68	0
2	PO4	B	603	-	4,4,4	1.20	0	6,6,6	0.61	0
2	PO4	D	606	-	4,4,4	1.02	0	6,6,6	0.48	0
2	PO4	B	612	-	4,4,4	0.83	0	6,6,6	0.60	0
2	PO4	B	609	-	4,4,4	0.94	0	6,6,6	0.55	0
2	PO4	C	611	-	4,4,4	0.93	0	6,6,6	0.66	0
3	GOL	C	701	-	5,5,5	0.34	0	5,5,5	0.37	0
2	PO4	C	605	-	4,4,4	0.94	0	6,6,6	0.62	0
2	PO4	C	608	-	4,4,4	0.83	0	6,6,6	0.57	0
2	PO4	D	602	-	4,4,4	0.87	0	6,6,6	0.51	0
3	GOL	B	702	-	5,5,5	0.35	0	5,5,5	0.31	0
2	PO4	A	604	-	4,4,4	0.92	0	6,6,6	0.57	0
2	PO4	A	610	-	4,4,4	1.00	0	6,6,6	0.54	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	GOL	C	701	-	-	2/4/4/4	-
3	GOL	B	702	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	GOL	C1-C2-C3-O3
3	C	701	GOL	O2-C2-C3-O3
3	B	702	GOL	O1-C1-C2-C3
3	C	701	GOL	C1-C2-C3-O3
3	B	702	GOL	O2-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	GOL	3	0
2	D	602	PO4	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	420/462 (90%)	0.34	37 (8%)	10 9	17, 35, 75, 92	0
1	B	420/462 (90%)	0.31	32 (7%)	13 13	19, 35, 73, 95	0
1	C	417/462 (90%)	0.23	26 (6%)	20 19	17, 33, 68, 97	0
1	D	420/462 (90%)	0.27	27 (6%)	19 18	19, 35, 69, 88	0
All	All	1677/1848 (90%)	0.29	122 (7%)	15 14	17, 34, 71, 97	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	GLY	9.9
1	A	116	LEU	7.2
1	A	456	VAL	6.9
1	C	116	LEU	6.6
1	B	116	LEU	5.9
1	A	380	ASN	5.8
1	C	22	LEU	5.5
1	D	448	ALA	5.2
1	C	33	SER	5.1
1	A	448	ALA	5.0
1	A	408	ARG	4.7
1	A	370	GLU	4.6
1	A	447	SER	4.5
1	A	444	PRO	4.5
1	B	380	ASN	4.3
1	C	445	GLY	4.2
1	C	56	SER	4.2
1	D	116	LEU	4.0
1	A	379	LEU	4.0
1	B	34	ASP	3.9
1	B	444	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	408	ARG	3.8
1	B	312	ALA	3.8
1	C	380	ASN	3.7
1	B	32	SER	3.7
1	C	60	LEU	3.7
1	B	412	ARG	3.6
1	B	59	LEU	3.6
1	C	129[A]	HIS	3.5
1	D	380	ASN	3.5
1	D	422	PRO	3.5
1	D	379	LEU	3.4
1	C	15	SER	3.4
1	D	59	LEU	3.4
1	A	430	GLN	3.3
1	D	412	ARG	3.3
1	C	62	LYS	3.3
1	A	449	TYR	3.2
1	B	128	THR	3.1
1	A	129	HIS	3.1
1	C	57	LYS	3.1
1	C	5	SER	3.1
1	B	61	ASP	3.0
1	B	86	GLU	3.0
1	A	412	ARG	3.0
1	B	127	ALA	3.0
1	C	422	PRO	3.0
1	C	58	GLU	2.9
1	B	15	SER	2.9
1	C	64	LYS	2.9
1	A	416	PHE	2.9
1	B	370	GLU	2.8
1	B	447	SER	2.8
1	C	417	GLU	2.8
1	A	413	HIS	2.8
1	B	115	HIS	2.8
1	D	57	LYS	2.8
1	A	366[A]	GLU	2.8
1	D	64	LYS	2.7
1	C	456	VAL	2.7
1	A	32	SER	2.7
1	A	443	LEU	2.7
1	D	455	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	417	GLU	2.7
1	B	311[A]	GLU	2.6
1	C	29	LYS	2.6
1	C	34	ASP	2.6
1	A	411	GLU	2.6
1	D	423	VAL	2.6
1	B	64	LYS	2.6
1	B	33	SER	2.6
1	D	34	ASP	2.6
1	A	59	LEU	2.6
1	B	405	GLU	2.6
1	C	416	PHE	2.5
1	C	115	HIS	2.5
1	D	117	ALA	2.4
1	A	397	VAL	2.4
1	A	15	SER	2.4
1	B	56	SER	2.4
1	D	30	THR	2.4
1	C	126	ASN	2.4
1	D	311	GLU	2.4
1	D	33	SER	2.4
1	D	374	ASN	2.4
1	D	363	LEU	2.3
1	A	30	THR	2.3
1	A	374	ASN	2.3
1	B	129	HIS	2.3
1	B	417	GLU	2.3
1	A	405	GLU	2.3
1	A	57	LYS	2.3
1	A	450	GLU	2.3
1	C	366[A]	GLU	2.3
1	B	363	LEU	2.3
1	B	346	GLU	2.2
1	B	12	PRO	2.2
1	C	370	GLU	2.2
1	C	55	ASN	2.2
1	D	370	GLU	2.2
1	A	62	LYS	2.2
1	C	246	ALA	2.2
1	D	87	HIS	2.2
1	B	445	GLY	2.2
1	A	61	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	424	LEU	2.1
1	A	311	GLU	2.1
1	D	164	VAL	2.1
1	A	53	THR	2.1
1	A	54	ASP	2.1
1	D	15	SER	2.1
1	D	388	ALA	2.1
1	B	450	GLU	2.1
1	B	87	HIS	2.1
1	D	366[A]	GLU	2.1
1	D	129	HIS	2.0
1	B	408	ARG	2.0
1	B	60	LEU	2.0
1	B	379	LEU	2.0
1	A	5	SER	2.0
1	D	62	LYS	2.0
1	A	393	ALA	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	GOL	C	701	6/6	0.80	0.19	32,44,52,55	0
3	GOL	B	702	6/6	0.88	0.14	57,67,69,78	0
2	PO4	B	612	5/5	0.89	0.21	55,62,71,72	0
2	PO4	B	607	5/5	0.90	0.19	32,60,65,71	0
2	PO4	C	611	5/5	0.95	0.10	42,57,60,65	0
2	PO4	C	608	5/5	0.96	0.15	47,52,55,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	B	609	5/5	0.96	0.18	57,58,69,69	0
2	PO4	A	610	5/5	0.97	0.13	55,55,65,68	0
2	PO4	D	602	5/5	0.98	0.19	35,44,55,57	0
2	PO4	D	606	5/5	0.98	0.24	55,63,66,68	0
2	PO4	C	605	5/5	0.99	0.04	23,25,30,35	0
2	PO4	B	603	5/5	0.99	0.07	16,20,25,28	0
2	PO4	A	604	5/5	0.99	0.04	22,22,28,28	0
2	PO4	D	601	5/5	0.99	0.07	28,28,29,37	0

6.5 Other polymers (i)

There are no such residues in this entry.