



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:58 PM UTC

PDB ID : 8BDQ / pdb_00008bdq
Title : Crystal structure of Bacteroides ovatus CP926 PL38 alginate lyase
Authors : Roenne, M.E.; Tandrup, T.; Wilkens, C.
Deposited on : 2022-10-19
Resolution : 2.11 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

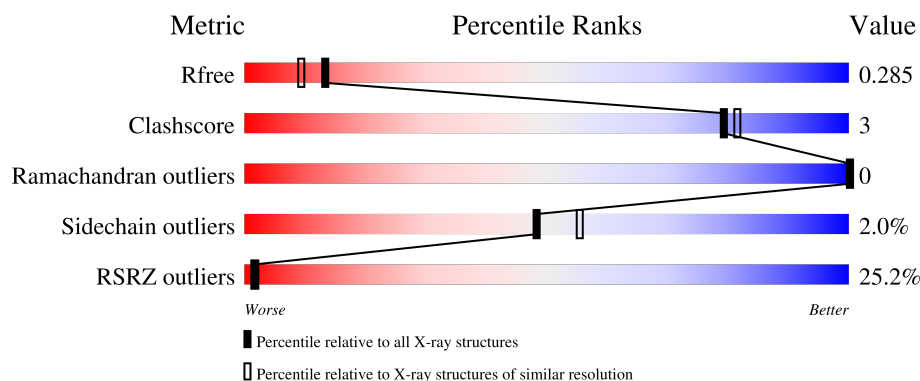
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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 $\leq 5\%$. 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	404	28% 85% 8% 6%
1	B	404	26% 85% 9% 6%
1	C	404	20% 88% 6% 6%
1	D	404	21% 84% 10% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12356 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 Alginate lyase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	1	0
			3055	1954	517	571	13			
1	B	380	Total	C	N	O	S	0	1	0
			3061	1957	518	573	13			
1	C	380	Total	C	N	O	S	0	2	0
			3069	1962	519	574	14			
1	D	381	Total	C	N	O	S	0	1	0
			3066	1960	519	574	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5M5BWR5
A	2	GLY	-	expression tag	UNP A0A5M5BWR5
A	3	SER	-	expression tag	UNP A0A5M5BWR5
A	4	SER	-	expression tag	UNP A0A5M5BWR5
A	5	HIS	-	expression tag	UNP A0A5M5BWR5
A	6	HIS	-	expression tag	UNP A0A5M5BWR5
A	7	HIS	-	expression tag	UNP A0A5M5BWR5
A	8	HIS	-	expression tag	UNP A0A5M5BWR5
A	9	HIS	-	expression tag	UNP A0A5M5BWR5
A	10	HIS	-	expression tag	UNP A0A5M5BWR5
A	11	SER	-	expression tag	UNP A0A5M5BWR5
A	12	SER	-	expression tag	UNP A0A5M5BWR5
A	13	GLY	-	expression tag	UNP A0A5M5BWR5
A	14	LEU	-	expression tag	UNP A0A5M5BWR5
A	15	VAL	-	expression tag	UNP A0A5M5BWR5
A	16	PRO	-	expression tag	UNP A0A5M5BWR5
A	17	ARG	-	expression tag	UNP A0A5M5BWR5
A	18	GLY	-	expression tag	UNP A0A5M5BWR5
A	19	SER	-	expression tag	UNP A0A5M5BWR5
A	20	HIS	-	expression tag	UNP A0A5M5BWR5
A	21	MET	-	expression tag	UNP A0A5M5BWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A5M5BWR5
A	23	SER	-	expression tag	UNP A0A5M5BWR5
B	1	MET	-	initiating methionine	UNP A0A5M5BWR5
B	2	GLY	-	expression tag	UNP A0A5M5BWR5
B	3	SER	-	expression tag	UNP A0A5M5BWR5
B	4	SER	-	expression tag	UNP A0A5M5BWR5
B	5	HIS	-	expression tag	UNP A0A5M5BWR5
B	6	HIS	-	expression tag	UNP A0A5M5BWR5
B	7	HIS	-	expression tag	UNP A0A5M5BWR5
B	8	HIS	-	expression tag	UNP A0A5M5BWR5
B	9	HIS	-	expression tag	UNP A0A5M5BWR5
B	10	HIS	-	expression tag	UNP A0A5M5BWR5
B	11	SER	-	expression tag	UNP A0A5M5BWR5
B	12	SER	-	expression tag	UNP A0A5M5BWR5
B	13	GLY	-	expression tag	UNP A0A5M5BWR5
B	14	LEU	-	expression tag	UNP A0A5M5BWR5
B	15	VAL	-	expression tag	UNP A0A5M5BWR5
B	16	PRO	-	expression tag	UNP A0A5M5BWR5
B	17	ARG	-	expression tag	UNP A0A5M5BWR5
B	18	GLY	-	expression tag	UNP A0A5M5BWR5
B	19	SER	-	expression tag	UNP A0A5M5BWR5
B	20	HIS	-	expression tag	UNP A0A5M5BWR5
B	21	MET	-	expression tag	UNP A0A5M5BWR5
B	22	ALA	-	expression tag	UNP A0A5M5BWR5
B	23	SER	-	expression tag	UNP A0A5M5BWR5
C	1	MET	-	initiating methionine	UNP A0A5M5BWR5
C	2	GLY	-	expression tag	UNP A0A5M5BWR5
C	3	SER	-	expression tag	UNP A0A5M5BWR5
C	4	SER	-	expression tag	UNP A0A5M5BWR5
C	5	HIS	-	expression tag	UNP A0A5M5BWR5
C	6	HIS	-	expression tag	UNP A0A5M5BWR5
C	7	HIS	-	expression tag	UNP A0A5M5BWR5
C	8	HIS	-	expression tag	UNP A0A5M5BWR5
C	9	HIS	-	expression tag	UNP A0A5M5BWR5
C	10	HIS	-	expression tag	UNP A0A5M5BWR5
C	11	SER	-	expression tag	UNP A0A5M5BWR5
C	12	SER	-	expression tag	UNP A0A5M5BWR5
C	13	GLY	-	expression tag	UNP A0A5M5BWR5
C	14	LEU	-	expression tag	UNP A0A5M5BWR5
C	15	VAL	-	expression tag	UNP A0A5M5BWR5
C	16	PRO	-	expression tag	UNP A0A5M5BWR5
C	17	ARG	-	expression tag	UNP A0A5M5BWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP A0A5M5BWR5
C	19	SER	-	expression tag	UNP A0A5M5BWR5
C	20	HIS	-	expression tag	UNP A0A5M5BWR5
C	21	MET	-	expression tag	UNP A0A5M5BWR5
C	22	ALA	-	expression tag	UNP A0A5M5BWR5
C	23	SER	-	expression tag	UNP A0A5M5BWR5
D	1	MET	-	initiating methionine	UNP A0A5M5BWR5
D	2	GLY	-	expression tag	UNP A0A5M5BWR5
D	3	SER	-	expression tag	UNP A0A5M5BWR5
D	4	SER	-	expression tag	UNP A0A5M5BWR5
D	5	HIS	-	expression tag	UNP A0A5M5BWR5
D	6	HIS	-	expression tag	UNP A0A5M5BWR5
D	7	HIS	-	expression tag	UNP A0A5M5BWR5
D	8	HIS	-	expression tag	UNP A0A5M5BWR5
D	9	HIS	-	expression tag	UNP A0A5M5BWR5
D	10	HIS	-	expression tag	UNP A0A5M5BWR5
D	11	SER	-	expression tag	UNP A0A5M5BWR5
D	12	SER	-	expression tag	UNP A0A5M5BWR5
D	13	GLY	-	expression tag	UNP A0A5M5BWR5
D	14	LEU	-	expression tag	UNP A0A5M5BWR5
D	15	VAL	-	expression tag	UNP A0A5M5BWR5
D	16	PRO	-	expression tag	UNP A0A5M5BWR5
D	17	ARG	-	expression tag	UNP A0A5M5BWR5
D	18	GLY	-	expression tag	UNP A0A5M5BWR5
D	19	SER	-	expression tag	UNP A0A5M5BWR5
D	20	HIS	-	expression tag	UNP A0A5M5BWR5
D	21	MET	-	expression tag	UNP A0A5M5BWR5
D	22	ALA	-	expression tag	UNP A0A5M5BWR5
D	23	SER	-	expression tag	UNP A0A5M5BWR5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

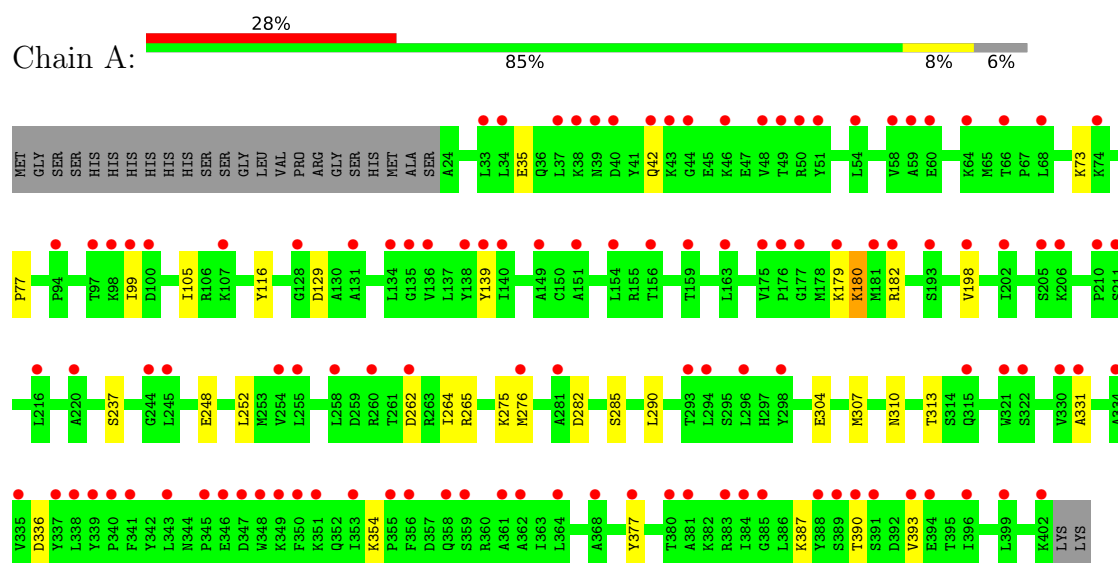
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	21	Total	O	0	0
			21	21		
3	C	21	Total	O	0	0
			21	21		
3	D	20	Total	O	0	0
			20	20		

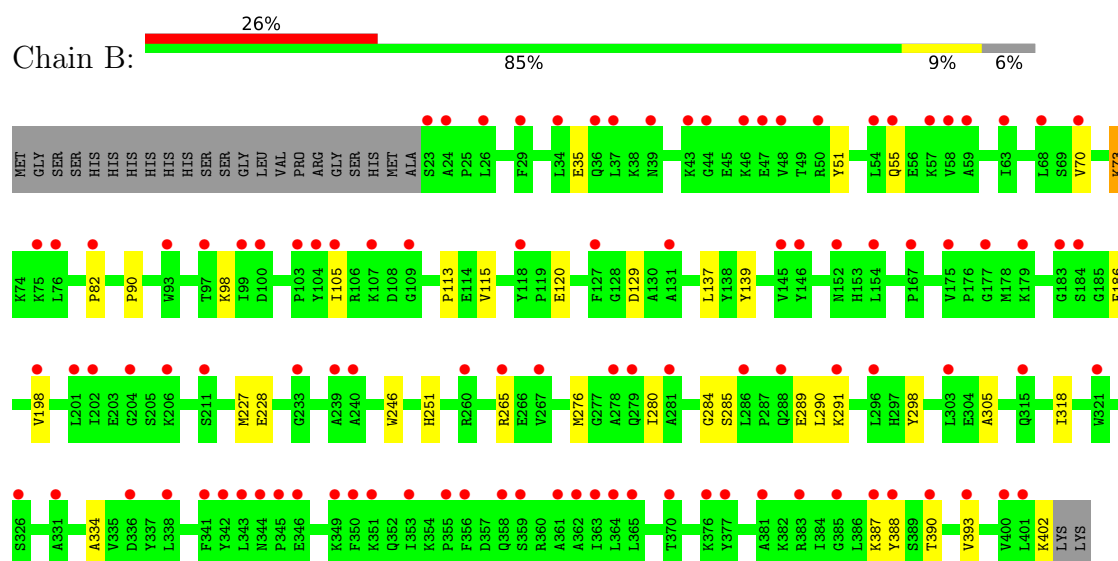
3 Residue-property plots

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: Alginate lyase family protein

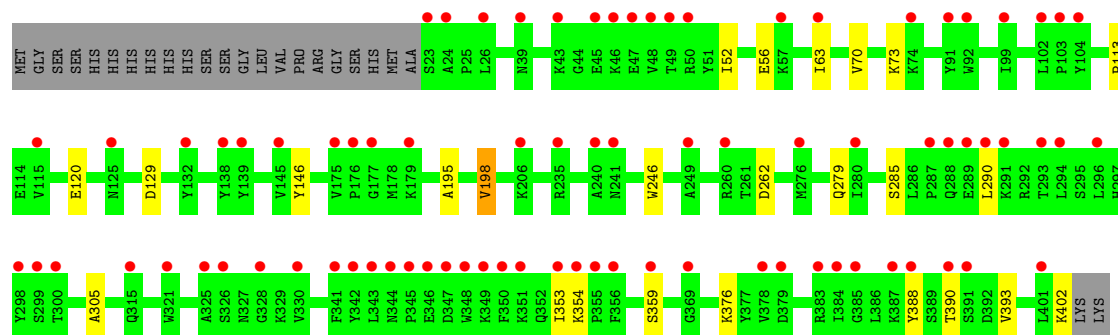


- Molecule 1: Alginate lyase family protein



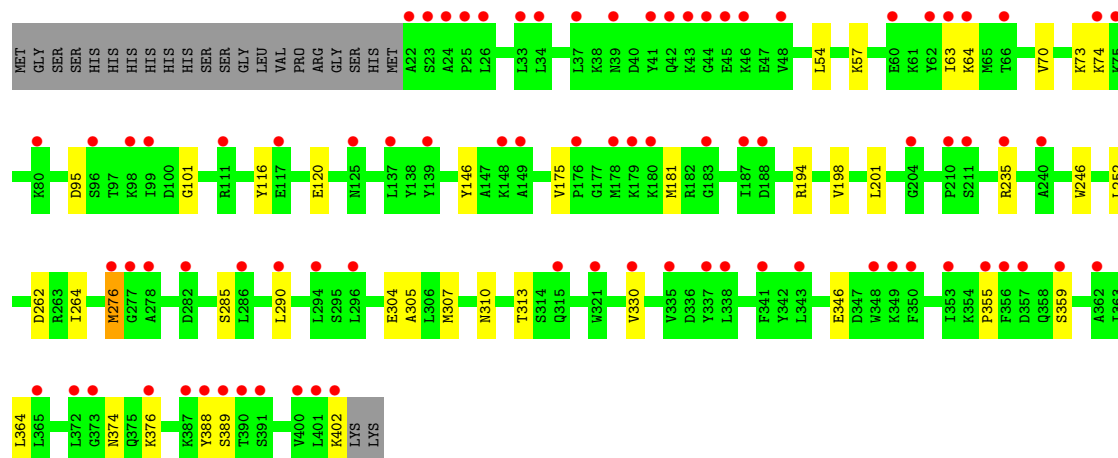
- Molecule 1: Alginate lyase family protein

Chain C: 



• Molecule 1: Alginate lyase family protein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.70Å 88.09Å 144.00Å 90.00° 120.06° 90.00°	Depositor
Resolution (Å)	48.12 – 2.11 48.12 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.12-2.11) 99.2 (48.12-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.12Å)	Xtriage
Refinement program	REFMAC 8.0, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.255 , 0.281 0.260 , 0.285	Depositor DCC
R_{free} test set	2101 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12356	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.79% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/3133	0.33	0/4246
1	B	0.15	0/3139	0.33	0/4254
1	C	0.14	0/3147	0.33	0/4264
1	D	0.14	0/3144	0.32	0/4261
All	All	0.14	0/12563	0.33	0/17025

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	3055	0	3024	16	0
1	B	3061	0	3029	19	0
1	C	3069	0	3037	13	0
1	D	3066	0	3034	20	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	0	0	0
3	C	21	0	0	1	0
3	D	20	0	0	0	0
All	All	12356	0	12124	65	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 (65) 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:35:GLU:OE2	1:B:139:TYR:OH	2.12	0.67
1:B:387:LYS:HB2	1:B:390:THR:HG23	1.85	0.58
1:A:336:ASP:OD1	1:A:377:TYR:OH	2.18	0.57
1:D:276:MET:HE3	1:D:330:VAL:HA	1.87	0.55
1:B:276:MET:HE3	1:B:280:ILE:HD11	1.89	0.55
1:C:195:ALA:O	1:C:198:VAL:HG12	2.08	0.54
1:A:180:LYS:HE3	1:A:180:LYS:H	1.72	0.54
1:A:262:ASP:OD1	1:A:265:ARG:NH1	2.40	0.54
1:D:54:LEU:HD21	1:D:389:SER:HA	1.89	0.54
1:D:285:SER:HB2	1:D:290:LEU:HD11	1.90	0.53
1:C:353:ILE:HB	1:D:355:PRO:HD3	1.89	0.53
1:A:35:GLU:OE2	1:A:139:TYR:OH	2.24	0.52
1:D:252:LEU:HD22	1:D:264:ILE:HG23	1.92	0.51
1:B:70:VAL:HG23	1:B:120:GLU:HG2	1.93	0.50
1:C:70:VAL:HG23	1:C:120:GLU:HG2	1.93	0.50
1:D:307:MET:HE2	1:D:364:LEU:HD13	1.94	0.49
1:C:279:GLN:NE2	3:C:601:HOH:O	2.35	0.49
1:B:73:LYS:HD2	1:B:82:PRO:HA	1.96	0.48
1:B:388:TYR:HA	1:B:402:LYS:HB3	1.95	0.48
1:A:276:MET:SD	1:A:331:ALA:HB2	2.53	0.48
1:B:228:GLU:OE2	1:B:251:HIS:NE2	2.44	0.47
1:A:129:ASP:HA	1:A:393:VAL:HG21	1.97	0.47
1:A:252:LEU:HD22	1:A:264:ILE:HG23	1.95	0.47
1:D:181:MET:O	1:D:235:ARG:NH1	2.47	0.46
1:B:186:PHE:CZ	1:B:227:MET:HE3	2.52	0.45
1:B:285:SER:HB2	1:B:290:LEU:HD11	1.99	0.44
1:D:70:VAL:HG23	1:D:120:GLU:HG2	2.00	0.44
1:A:73:LYS:HE3	1:A:77:PRO:HD3	1.98	0.44
1:D:63:ILE:HD11	1:D:146:TYR:CE1	2.53	0.44
1:C:353:ILE:HG13	1:C:354:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TRP:CE2	1:B:305:ALA:HB2	2.53	0.44
1:C:52:ILE:O	1:C:56:GLU:HG3	2.18	0.44
1:D:95:ASP:O	1:D:101:GLY:HA2	2.17	0.44
1:A:248:GLU:HA	1:A:248:GLU:OE1	2.17	0.44
1:A:237:SER:O	1:A:275:LYS:NZ	2.32	0.44
1:A:304:GLU:HA	1:A:307:MET:HE2	1.99	0.43
1:A:285:SER:HB2	1:A:290:LEU:HD11	1.99	0.43
1:A:387:LYS:HB2	1:A:390:THR:HG23	2.00	0.43
1:C:129:ASP:HA	1:C:393:VAL:HG21	1.99	0.43
1:B:129:ASP:HA	1:B:393:VAL:HG21	2.00	0.43
1:A:354:LYS:HB3	1:A:354:LYS:HE2	1.86	0.43
1:C:246:TRP:CD1	1:C:305:ALA:HB2	2.54	0.43
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.83	0.43
1:D:198:VAL:HG13	1:D:201:LEU:HD12	2.01	0.42
1:B:90:PRO:HA	1:B:115:VAL:HG11	2.01	0.42
1:B:284:GLY:O	1:B:334:ALA:HA	2.19	0.42
1:D:374:ASN:OD1	1:D:376:LYS:HG2	2.20	0.42
1:B:98:LYS:HB3	1:B:98:LYS:HE2	1.81	0.42
1:D:262:ASP:N	1:D:262:ASP:OD1	2.53	0.42
1:C:113:PRO:HB3	1:D:116:TYR:CZ	2.55	0.42
1:B:265:ARG:HG3	1:B:318:ILE:HD11	2.01	0.42
1:C:63:ILE:HD11	1:C:146:TYR:CE1	2.55	0.42
1:A:116:TYR:CZ	1:B:113:PRO:HB3	2.55	0.41
1:D:388:TYR:HA	1:D:402:LYS:HB3	2.02	0.41
1:D:304:GLU:HA	1:D:307:MET:HE3	2.02	0.41
1:B:51:TYR:O	1:B:55:GLN:HG2	2.20	0.41
1:D:70:VAL:CG2	1:D:120:GLU:HG2	2.51	0.41
1:D:194:ARG:O	1:D:198:VAL:HG23	2.20	0.41
1:D:246:TRP:CD1	1:D:305:ALA:HB2	2.56	0.41
1:C:388:TYR:HA	1:C:402:LYS:HB3	2.03	0.41
1:C:285:SER:HB2	1:C:290:LEU:HD11	2.03	0.40
1:A:310:ASN:HA	1:A:313:THR:OG1	2.22	0.40
1:D:310:ASN:HA	1:D:313:THR:OG1	2.21	0.40
1:B:289:GLU:OE1	1:B:298:TYR:HB3	2.22	0.40
1:C:246:TRP:CE2	1:C:305:ALA:HB2	2.57	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	378/404 (94%)	370 (98%)	8 (2%)	0	100	100
1	B	379/404 (94%)	369 (97%)	10 (3%)	0	100	100
1	C	380/404 (94%)	373 (98%)	7 (2%)	0	100	100
1	D	380/404 (94%)	373 (98%)	7 (2%)	0	100	100
All	All	1517/1616 (94%)	1485 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	324/344 (94%)	316 (98%)	8 (2%)	42	47
1	B	325/344 (94%)	321 (99%)	4 (1%)	63	71
1	C	326/344 (95%)	320 (98%)	6 (2%)	51	59
1	D	325/344 (94%)	317 (98%)	8 (2%)	42	47
All	All	1300/1376 (94%)	1274 (98%)	26 (2%)	48	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	99	ILE

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Mol	Chain	Res	Type
1	A	105	ILE
1	A	179	LYS
1	A	180	LYS
1	A	182	ARG
1	A	198	VAL
1	A	282	ASP
1	B	73	LYS
1	B	105	ILE
1	B	198	VAL
1	B	291	LYS
1	C	73	LYS
1	C	198	VAL
1	C	262	ASP
1	C	359	SER
1	C	376	LYS
1	C	390	THR
1	D	57	LYS
1	D	64	LYS
1	D	73	LYS
1	D	74	LYS
1	D	175	VAL
1	D	276	MET
1	D	346	GLU
1	D	359	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	B	242	ASN
1	B	270	GLN
1	B	279	GLN
1	B	358	GLN
1	B	375	GLN
1	C	358	GLN
1	D	125	ASN
1	D	234	GLN
1	D	279	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	501	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	502	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	D	501	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	379/404 (93%)	1.58	114 (30%) 1 1	26, 51, 71, 86	1 (0%)
1	B	380/404 (94%)	1.52	104 (27%) 1 1	24, 50, 70, 93	1 (0%)
1	C	380/404 (94%)	1.46	82 (21%) 2 2	26, 51, 72, 105	2 (0%)
1	D	381/404 (94%)	1.40	83 (21%) 2 2	25, 51, 72, 116	1 (0%)
All	All	1520/1616 (94%)	1.49	383 (25%) 1 2	24, 51, 72, 116	5 (0%)

All (383) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	8.7
1	A	349	LYS	5.4
1	D	23	SER	5.4
1	C	315[A]	GLN	5.3
1	C	23	SER	5.3
1	A	353	ILE	5.3
1	B	48	VAL	5.1
1	D	276	MET	4.8
1	B	99	ILE	4.7
1	C	348	TRP	4.7
1	C	354	LYS	4.7
1	C	325	ALA	4.6
1	C	343	LEU	4.3
1	D	99	ILE	4.3
1	D	349	LYS	4.3
1	C	276[A]	MET	4.2
1	C	179	LYS	4.1
1	A	50	ARG	4.0
1	A	343	LEU	4.0
1	B	362	ALA	4.0
1	A	361	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	288	GLN	3.9
1	A	99	ILE	3.9
1	C	26	LEU	3.9
1	A	64	LYS	3.8
1	D	74	LYS	3.8
1	C	293	THR	3.8
1	B	46	LYS	3.8
1	D	44	GLY	3.7
1	A	48	VAL	3.7
1	A	74	LYS	3.7
1	D	315[A]	GLN	3.7
1	A	281	ALA	3.6
1	D	187	ILE	3.6
1	D	183	GLY	3.6
1	B	353	ILE	3.6
1	C	353	ILE	3.6
1	D	353	ILE	3.6
1	A	39	ASN	3.5
1	B	390	THR	3.5
1	B	381	ALA	3.5
1	C	50	ARG	3.5
1	D	355	PRO	3.5
1	B	359	SER	3.5
1	A	350	PHE	3.4
1	A	258	LEU	3.4
1	A	383	ARG	3.4
1	C	390	THR	3.4
1	A	210	PRO	3.4
1	B	76	LEU	3.4
1	B	321	TRP	3.4
1	B	349	LYS	3.4
1	C	99	ILE	3.4
1	C	74	LYS	3.3
1	B	58	VAL	3.3
1	B	201	LEU	3.3
1	C	355	PRO	3.2
1	B	37	LEU	3.2
1	A	60	GLU	3.2
1	D	46	LYS	3.2
1	B	350	PHE	3.2
1	C	45	GLU	3.1
1	B	370	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	206	LYS	3.1
1	A	355	PRO	3.1
1	B	315[A]	GLN	3.1
1	B	34	LEU	3.1
1	A	46	LYS	3.1
1	C	145	VAL	3.1
1	C	175	VAL	3.1
1	C	321	TRP	3.1
1	C	326	SER	3.1
1	D	45	GLU	3.1
1	D	34	LEU	3.1
1	D	63	ILE	3.1
1	B	23	SER	3.1
1	D	388	TYR	3.0
1	C	341	PHE	3.0
1	D	356	PHE	3.0
1	A	206	LYS	3.0
1	A	335	VAL	3.0
1	B	145	VAL	3.0
1	C	350	PHE	3.0
1	D	282	ASP	3.0
1	D	64	LYS	3.0
1	B	63	ILE	3.0
1	B	345	PRO	3.0
1	B	326	SER	3.0
1	C	115	VAL	3.0
1	A	331	ALA	2.9
1	B	211	SER	2.9
1	C	346	GLU	2.9
1	D	188	ASP	2.9
1	A	337	TYR	2.9
1	C	349	LYS	2.9
1	D	296	LEU	2.9
1	B	204	GLY	2.9
1	B	68	LEU	2.9
1	B	177	GLY	2.9
1	D	48	VAL	2.9
1	D	330	VAL	2.9
1	C	235	ARG	2.9
1	D	373	GLY	2.9
1	A	54	LEU	2.8
1	D	343	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	400	VAL	2.8
1	C	356	PHE	2.8
1	D	24	ALA	2.8
1	C	294	LEU	2.8
1	A	384	ILE	2.8
1	B	351	LYS	2.8
1	C	351	LYS	2.8
1	A	358	GLN	2.8
1	A	40	ASP	2.8
1	B	356	PHE	2.8
1	A	321	TRP	2.8
1	A	276	MET	2.8
1	A	151	ALA	2.8
1	B	146	TYR	2.8
1	D	376	LYS	2.8
1	D	390	THR	2.8
1	A	254	VAL	2.8
1	C	347	ASP	2.7
1	A	135	GLY	2.7
1	A	179	LYS	2.7
1	B	24	ALA	2.7
1	B	240	ALA	2.7
1	A	346	GLU	2.7
1	A	149	ALA	2.7
1	D	137	LEU	2.7
1	A	138	TYR	2.7
1	C	138	TYR	2.7
1	A	347	ASP	2.7
1	D	148	LYS	2.7
1	B	54	LEU	2.7
1	A	345	PRO	2.7
1	C	39	ASN	2.7
1	D	389	SER	2.7
1	B	279	GLN	2.6
1	C	47	GLU	2.6
1	A	390	THR	2.6
1	D	341	PHE	2.6
1	C	296	LEU	2.6
1	C	103	PRO	2.6
1	B	43	LYS	2.6
1	D	321	TRP	2.6
1	A	340	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	2.6
1	B	103	PRO	2.6
1	B	154	LEU	2.6
1	B	364	LEU	2.6
1	D	210	PRO	2.6
1	D	338	LEU	2.6
1	B	105	ILE	2.6
1	C	385	GLY	2.6
1	C	24	ALA	2.6
1	B	26	LEU	2.6
1	C	290	LEU	2.6
1	B	341	PHE	2.6
1	A	339	TYR	2.6
1	D	62	TYR	2.6
1	D	39	ASN	2.6
1	B	291	LYS	2.6
1	C	46	LYS	2.6
1	A	49	THR	2.6
1	A	362	ALA	2.6
1	D	362	ALA	2.6
1	A	364	LEU	2.6
1	C	102	LEU	2.6
1	C	401	LEU	2.6
1	B	206	LYS	2.5
1	C	344	ASN	2.5
1	D	42	GLN	2.5
1	B	29	PHE	2.5
1	B	387	LYS	2.5
1	A	334	ALA	2.5
1	A	391	SER	2.5
1	B	331	ALA	2.5
1	C	176	PRO	2.5
1	C	287	PRO	2.5
1	B	401	LEU	2.5
1	A	341	PHE	2.5
1	A	356	PHE	2.5
1	B	127	PHE	2.5
1	B	57	LYS	2.5
1	D	43	LYS	2.5
1	A	42	GLN	2.5
1	A	66	THR	2.5
1	D	149	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	240	ALA	2.5
1	A	33	LEU	2.5
1	B	343	LEU	2.5
1	B	179	LYS	2.5
1	A	381	ALA	2.4
1	D	26	LEU	2.4
1	D	180	LYS	2.4
1	D	365	LEU	2.4
1	D	125	ASN	2.4
1	A	198	VAL	2.4
1	A	139	TYR	2.4
1	A	389	SER	2.4
1	C	298	TYR	2.4
1	D	359	SER	2.4
1	B	50	ARG	2.4
1	B	361	ALA	2.4
1	D	235	ARG	2.4
1	D	387	LYS	2.4
1	A	245	LEU	2.4
1	A	294	LEU	2.4
1	B	338	LEU	2.4
1	D	33	LEU	2.4
1	A	315[A]	GLN	2.4
1	D	335	VAL	2.4
1	A	348	TRP	2.4
1	D	66	THR	2.4
1	B	82	PRO	2.4
1	B	286	LEU	2.4
1	A	44	GLY	2.4
1	D	277	GLY	2.4
1	B	70	VAL	2.4
1	B	202	ILE	2.4
1	A	156	THR	2.4
1	D	41	TYR	2.3
1	B	346	GLU	2.3
1	A	154	LEU	2.3
1	A	100	ASP	2.3
1	D	98	LYS	2.3
1	B	363	ILE	2.3
1	C	48	VAL	2.3
1	A	377	TYR	2.3
1	A	128	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	296	LEU	2.3
1	C	383	ARG	2.3
1	B	75	LYS	2.3
1	D	75	LYS	2.3
1	C	280	ILE	2.3
1	B	393	VAL	2.3
1	D	60	GLU	2.3
1	A	380	THR	2.3
1	D	278	ALA	2.3
1	A	34	LEU	2.3
1	A	388	TYR	2.3
1	B	388	TYR	2.3
1	C	388	TYR	2.3
1	A	43	LYS	2.3
1	A	211	SER	2.3
1	D	350	PHE	2.3
1	A	140	ILE	2.3
1	B	36	GLN	2.3
1	A	175	VAL	2.3
1	A	351	LYS	2.3
1	A	402	LYS	2.3
1	B	107	LYS	2.3
1	B	131	ALA	2.3
1	C	43	LYS	2.3
1	B	377	TYR	2.3
1	C	289	GLU	2.2
1	C	299	SER	2.2
1	C	345	PRO	2.2
1	D	25	PRO	2.2
1	B	383	ARG	2.2
1	C	379	ASP	2.2
1	A	220	ALA	2.2
1	B	44	GLY	2.2
1	A	296	LEU	2.2
1	B	118	TYR	2.2
1	C	342	TYR	2.2
1	B	288	GLN	2.2
1	A	193	SER	2.2
1	A	205	SER	2.2
1	A	359	SER	2.2
1	D	211	SER	2.2
1	A	107	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	293	THR	2.2
1	C	387	LYS	2.2
1	D	179	LYS	2.2
1	B	281	ALA	2.2
1	D	286	LEU	2.2
1	D	290	LEU	2.2
1	D	294	LEU	2.2
1	D	139	TYR	2.2
1	B	184	SER	2.2
1	D	96	SER	2.2
1	A	98	LYS	2.2
1	A	396	ILE	2.2
1	D	176	PRO	2.2
1	A	177	GLY	2.2
1	C	249	ALA	2.2
1	B	93	TRP	2.2
1	C	378	VAL	2.1
1	B	183	GLY	2.1
1	B	59	ALA	2.1
1	A	68	LEU	2.1
1	A	134	LEU	2.1
1	D	37	LEU	2.1
1	D	111	ARG	2.1
1	C	359	SER	2.1
1	D	80	LYS	2.1
1	B	39	ASN	2.1
1	C	91	TYR	2.1
1	C	241	ASN	2.1
1	A	97	THR	2.1
1	B	355	PRO	2.1
1	C	92	TRP	2.1
1	D	348	TRP	2.1
1	B	358	GLN	2.1
1	C	384	ILE	2.1
1	B	198	VAL	2.1
1	C	328	GLY	2.1
1	C	330	VAL	2.1
1	A	182	ARG	2.1
1	A	260	ARG	2.1
1	C	260	ARG	2.1
1	C	240	ALA	2.1
1	A	255	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	57	LYS	2.1
1	C	391	SER	2.1
1	B	344	ASN	2.1
1	C	125	ASN	2.1
1	C	139	TYR	2.1
1	A	159	THR	2.1
1	A	176	PRO	2.1
1	B	97	THR	2.1
1	A	202	ILE	2.1
1	A	244	GLY	2.1
1	A	58	VAL	2.1
1	B	267	VAL	2.1
1	D	402	LYS	2.1
1	A	131	ALA	2.1
1	B	239	ALA	2.1
1	B	278	ALA	2.1
1	A	163	LEU	2.1
1	A	322	SER	2.1
1	B	303	LEU	2.1
1	D	401	LEU	2.1
1	A	181	MET	2.1
1	A	394	GLU	2.1
1	D	178	MET	2.1
1	B	152	ASN	2.1
1	B	100	ASP	2.1
1	A	94	PRO	2.1
1	B	104	TYR	2.1
1	B	260	ARG	2.1
1	B	265	ARG	2.1
1	C	104	TYR	2.1
1	C	300	THR	2.1
1	D	337	TYR	2.1
1	B	109	GLY	2.1
1	A	38	LYS	2.1
1	C	291	LYS	2.1
1	A	330	VAL	2.1
1	A	393	VAL	2.1
1	B	175	VAL	2.1
1	D	400	VAL	2.1
1	A	59	ALA	2.1
1	A	368	ALA	2.1
1	B	47	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	117	GLU	2.0
1	A	37	LEU	2.0
1	A	338	LEU	2.0
1	B	55	GLN	2.0
1	B	336	ASP	2.0
1	D	357	ASP	2.0
1	B	167	PRO	2.0
1	C	49	THR	2.0
1	A	298	TYR	2.0
1	A	385	GLY	2.0
1	C	132	TYR	2.0
1	D	204	GLY	2.0
1	C	63	ILE	2.0
1	A	136	VAL	2.0
1	D	391	SER	2.0
1	A	216	LEU	2.0
1	B	365	LEU	2.0
1	D	372	LEU	2.0
1	A	262	ASP	2.0
1	B	376	LYS	2.0
1	B	233	GLY	2.0
1	B	385	GLY	2.0
1	C	177	GLY	2.0
1	C	369	GLY	2.0
1	A	51	TYR	2.0
1	B	342	TYR	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	501	5/5	0.85	0.12	54,61,64,68	0
2	SO4	D	501	5/5	0.85	0.12	57,62,64,64	0
2	SO4	B	502	5/5	0.91	0.13	49,52,57,60	0
2	SO4	C	501	5/5	0.94	0.09	57,58,61,66	0
2	SO4	B	501	5/5	0.96	0.08	54,58,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.