



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2024 – 03:29 PM EDT

PDB ID : 8TEF
Title : PorX primitive monoclinic crystal form
Authors : Saran, A.; Zeytuni, N.
Deposited on : 2023-07-06
Resolution : 2.85 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.1
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) : 2.36.1

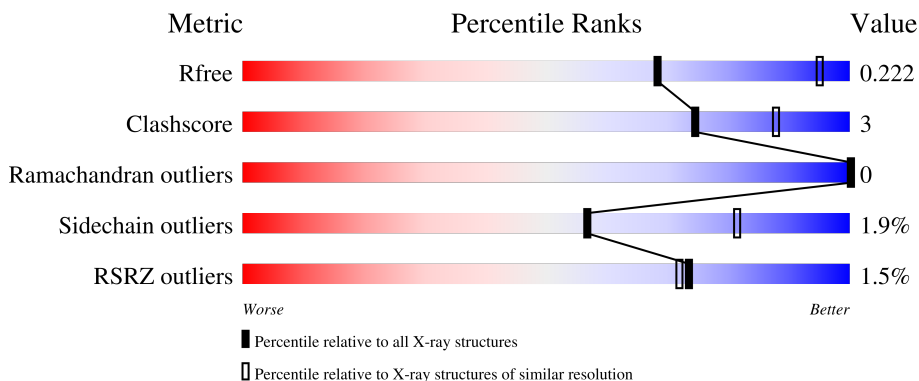
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	520	88% 11% .
1	B	520	91% 8% .
1	C	520	87% 9% .
1	D	520	89% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	604	-	-	X	-
2	SO4	D	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16912 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 Response regulator receiver protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	4248	2756	671	805	16	0	2	0
1	B	516	4243	2752	671	805	15	0	1	0
1	C	497	4098	2666	647	771	14	0	0	0
1	D	512	4208	2732	665	796	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A5FFU4
A	-1	SER	-	expression tag	UNP A5FFU4
A	0	HIS	-	expression tag	UNP A5FFU4
B	-2	GLY	-	expression tag	UNP A5FFU4
B	-1	SER	-	expression tag	UNP A5FFU4
B	0	HIS	-	expression tag	UNP A5FFU4
C	-2	GLY	-	expression tag	UNP A5FFU4
C	-1	SER	-	expression tag	UNP A5FFU4
C	0	HIS	-	expression tag	UNP A5FFU4
D	-2	GLY	-	expression tag	UNP A5FFU4
D	-1	SER	-	expression tag	UNP A5FFU4
D	0	HIS	-	expression tag	UNP A5FFU4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

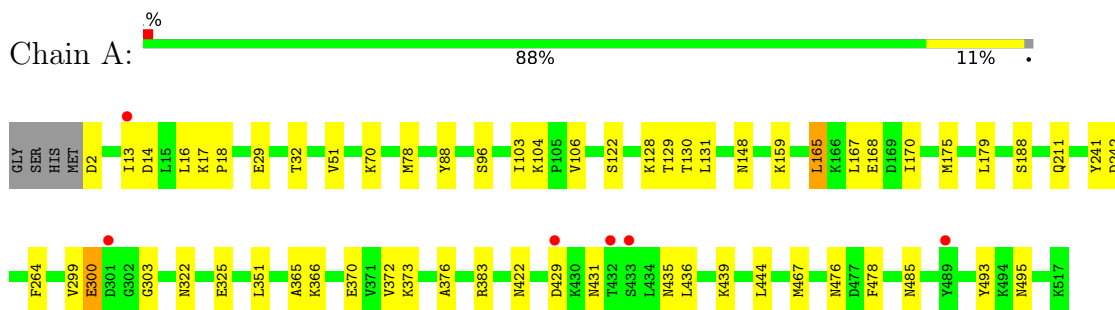
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O 27 27	0	0
4	B	18	Total O 18 18	0	0
4	C	4	Total O 4 4	0	0
4	D	7	Total O 7 7	0	0

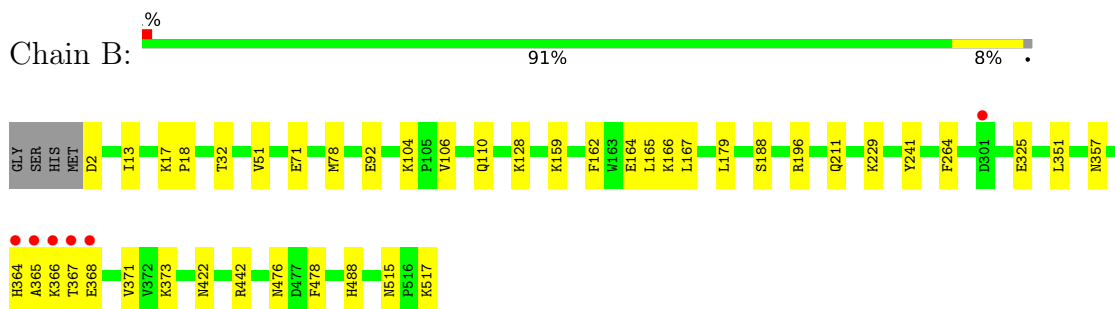
3 Residue-property plots [i](#)

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.

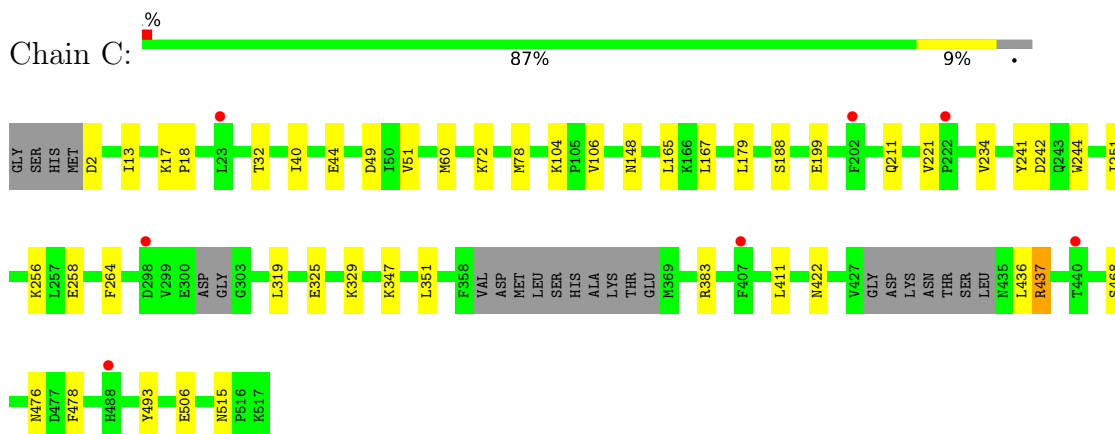
- Molecule 1: Response regulator receiver protein



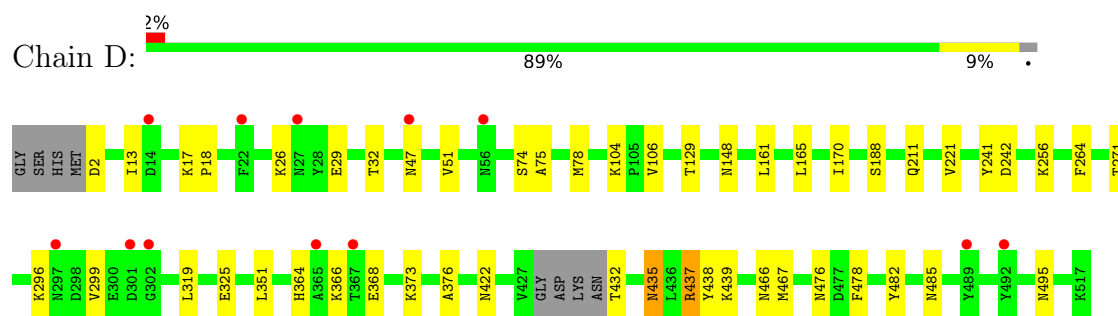
- Molecule 1: Response regulator receiver protein



- Molecule 1: Response regulator receiver protein



- Molecule 1: Response regulator receiver protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.52Å 57.52Å 149.14Å 90.00° 98.39° 90.00°	Depositor
Resolution (Å)	45.40 – 2.85 45.36 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.40-2.85) 99.1 (45.36-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.177 , 0.222 0.181 , 0.222	Depositor DCC
R_{free} test set	2644 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtrriage
Anisotropy	0.082	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16912	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.83% 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: MG, 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	0.36	0/4346	0.62	0/5867
1	B	0.37	0/4338	0.65	1/5857 (0.0%)
1	C	0.33	0/4186	0.63	1/5648 (0.0%)
1	D	0.34	0/4299	0.62	0/5804
All	All	0.35	0/17169	0.63	2/23176 (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	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	437	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	488	HIS	CB-CA-C	5.16	120.72	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	442	ARG	Sidechain
1	D	437	ARG	Sidechain

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	4248	0	4271	33	0
1	B	4243	0	4262	30	0
1	C	4098	0	4121	26	0
1	D	4208	0	4229	28	0
2	A	10	0	0	0	0
2	B	20	0	0	4	0
2	C	15	0	0	1	0
2	D	10	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	27	0	0	0	0
4	B	18	0	0	0	0
4	C	4	0	0	0	0
4	D	7	0	0	0	0
All	All	16912	0	16883	109	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 (109) 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:A:13:ILE:HD12	1:A:16:LEU:HD12	1.69	0.74
1:D:296:LYS:O	1:D:299:VAL:HG13	1.89	0.73
1:B:196:ARG:NH1	2:B:604:SO4:O1	2.24	0.71
1:D:432:THR:N	1:D:482:TYR:HH	1.90	0.69
1:A:13:ILE:HG12	1:A:32:THR:HB	1.75	0.69
1:A:435:ASN:O	1:A:439:LYS:NZ	2.26	0.68
1:D:366:LYS:O	1:D:373:LYS:HG3	1.94	0.67
1:D:435:ASN:O	1:D:439:LYS:NZ	2.28	0.66
1:A:159:LYS:HE2	1:B:71:GLU:OE2	1.96	0.64
1:A:366:LYS:NZ	1:A:495:ASN:O	2.31	0.63
1:A:429:ASP:HB3	1:A:444:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASN:ND2	2:B:603:SO4:O3	2.32	0.62
1:D:466:ASN:OD1	1:D:467:MET:N	2.32	0.62
1:A:103:ILE:H	1:B:110:GLN:HE22	1.47	0.62
1:D:271:THR:HB	2:D:601:SO4:O3	2.00	0.62
1:B:366:LYS:O	1:B:373:LYS:HG3	2.00	0.61
1:D:74:SER:O	1:D:75:ALA:HB3	2.00	0.61
1:B:366:LYS:HD2	1:B:373:LYS:HA	1.82	0.60
1:C:49:ASP:OD1	1:D:256:LYS:HD3	2.01	0.60
1:C:258:GLU:HG3	1:C:515:ASN:OD1	2.02	0.59
1:D:435:ASN:HD22	1:D:437:ARG:H	1.50	0.58
1:C:40:ILE:HD11	1:C:60:MET:HE1	1.85	0.58
1:D:366:LYS:NZ	1:D:495:ASN:O	2.37	0.57
1:D:188:SER:HA	1:D:476:ASN:HD21	1.69	0.57
1:A:188:SER:HA	1:A:476:ASN:HD21	1.70	0.56
1:A:300:GLU:H	1:A:300:GLU:CD	2.08	0.56
1:C:188:SER:HA	1:C:476:ASN:HD21	1.70	0.56
1:D:13:ILE:HG12	1:D:32:THR:HB	1.86	0.56
1:C:244:TRP:CZ3	1:C:251:ILE:HD11	2.41	0.56
1:C:437:ARG:NH1	1:C:506:GLU:OE1	2.39	0.55
1:B:364:HIS:O	1:B:367:THR:HG22	2.05	0.55
1:C:51:VAL:HB	1:C:78:MET:HG2	1.87	0.55
1:C:437:ARG:HD3	1:C:506:GLU:OE2	2.07	0.54
1:C:13:ILE:HG12	1:C:32:THR:HB	1.89	0.54
1:D:364:HIS:O	1:D:368:GLU:HG2	2.08	0.54
1:B:51:VAL:HB	1:B:78:MET:HG2	1.89	0.54
1:B:188:SER:HA	1:B:476:ASN:HD21	1.73	0.53
1:A:128:LYS:HE2	1:B:92:GLU:HG3	1.88	0.53
1:C:436:LEU:HD11	1:C:493:TYR:CG	2.44	0.52
1:A:13:ILE:CD1	1:A:16:LEU:HD12	2.39	0.52
1:B:196:ARG:NH1	2:B:604:SO4:S	2.82	0.52
1:B:162:PHE:CZ	1:B:166:LYS:HD2	2.45	0.52
1:D:188:SER:HA	1:D:476:ASN:ND2	2.25	0.51
1:A:211:GLN:HA	1:A:264:PHE:O	2.11	0.51
1:B:229:LYS:HE3	1:B:515:ASN:HD22	1.76	0.51
1:D:211:GLN:HA	1:D:264:PHE:O	2.11	0.51
1:B:17:LYS:N	1:B:18:PRO:CD	2.75	0.50
1:A:436:LEU:HD21	1:A:493:TYR:CG	2.46	0.50
1:B:211:GLN:HA	1:B:264:PHE:O	2.12	0.50
1:B:13:ILE:HG12	1:B:32:THR:HB	1.94	0.49
1:A:51:VAL:HB	1:A:78:MET:HG2	1.94	0.49
1:A:96:SER:OG	1:B:128:LYS:HE3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:GLN:HA	1:C:264:PHE:O	2.12	0.49
1:A:365:ALA:HB2	1:B:371:VAL:HG21	1.95	0.49
1:C:17:LYS:N	1:C:18:PRO:CD	2.77	0.48
1:C:44:GLU:HG3	1:C:72:LYS:HD3	1.96	0.48
1:D:366:LYS:HE3	1:D:376:ALA:O	2.13	0.48
1:A:17:LYS:N	1:A:18:PRO:CD	2.77	0.48
1:D:435:ASN:ND2	1:D:437:ARG:H	2.11	0.48
1:C:244:TRP:CH2	1:C:251:ILE:HD11	2.50	0.47
1:B:229:LYS:HE3	1:B:515:ASN:ND2	2.29	0.47
1:D:51:VAL:HB	1:D:78:MET:HG2	1.97	0.47
1:C:256:LYS:HE2	1:D:47:ASN:HB3	1.97	0.46
1:D:17:LYS:N	1:D:18:PRO:CD	2.79	0.46
1:A:104:LYS:HA	1:A:106:VAL:HG23	1.97	0.46
1:B:104:LYS:HA	1:B:106:VAL:HG23	1.98	0.46
1:C:258:GLU:CG	1:C:515:ASN:OD1	2.64	0.45
1:A:429:ASP:OD1	1:A:439:LYS:HD2	2.17	0.45
1:C:167:LEU:HD12	1:C:179:LEU:HD22	1.99	0.45
1:A:103:ILE:H	1:B:110:GLN:NE2	2.14	0.45
1:A:365:ALA:HB1	1:A:372:VAL:HG21	1.98	0.45
1:C:104:LYS:HA	1:C:106:VAL:HG23	1.99	0.45
1:B:167:LEU:HD12	1:B:179:LEU:HD22	1.98	0.45
1:D:271:THR:CB	2:D:601:SO4:O3	2.65	0.44
1:A:165:LEU:O	1:A:168:GLU:HB2	2.18	0.44
1:C:188:SER:HA	1:C:476:ASN:ND2	2.33	0.44
1:D:129:THR:HB	1:D:170:ILE:HD11	1.99	0.44
1:D:422:ASN:O	1:D:478:PHE:HA	2.18	0.44
1:D:325:GLU:HA	1:D:351:LEU:O	2.18	0.43
1:D:104:LYS:HA	1:D:106:VAL:HG23	1.99	0.43
1:A:167:LEU:HD22	1:A:179:LEU:HD22	2.00	0.43
1:A:299:VAL:HG21	1:A:303:GLY:O	2.18	0.43
1:C:329:LYS:HD2	2:C:603:SO4:O4	2.19	0.43
1:C:422:ASN:O	1:C:478:PHE:HA	2.19	0.43
1:A:175[B]:MET:HE3	1:A:175[B]:MET:HB3	1.87	0.42
1:A:325:GLU:HA	1:A:351:LEU:O	2.19	0.42
1:C:325:GLU:HA	1:C:351:LEU:O	2.18	0.42
1:A:188:SER:HA	1:A:476:ASN:ND2	2.32	0.42
1:B:188:SER:HA	1:B:476:ASN:ND2	2.33	0.42
1:A:70:LYS:HD3	1:A:78:MET:SD	2.59	0.42
1:C:221:VAL:HG21	1:C:319:LEU:HD13	2.02	0.42
1:B:164[A]:GLU:HA	1:B:179:LEU:HD21	2.00	0.42
1:B:159:LYS:HB2	1:B:159:LYS:HE2	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164[B]:GLU:HA	1:B:179:LEU:HD21	2.00	0.42
1:A:242:ASP:HB2	1:A:383:ARG:HD3	2.00	0.42
1:C:199:GLU:H	1:C:199:GLU:CD	2.23	0.42
1:C:242:ASP:HB2	1:C:383:ARG:HD3	2.02	0.42
1:B:325:GLU:HA	1:B:351:LEU:O	2.20	0.42
1:D:221:VAL:HG21	1:D:319:LEU:HD13	2.02	0.41
1:A:366:LYS:HE3	1:A:376:ALA:O	2.20	0.41
1:B:196:ARG:NH1	2:B:604:SO4:O3	2.52	0.41
1:D:74:SER:O	1:D:75:ALA:CB	2.66	0.41
1:A:129:THR:HB	1:A:170:ILE:HD11	2.02	0.41
1:B:422:ASN:O	1:B:478:PHE:HA	2.21	0.41
1:A:130:THR:OG1	1:A:170:ILE:HD12	2.21	0.41
1:C:234:VAL:HB	1:C:411:LEU:HD12	2.03	0.41
1:D:161:LEU:HD22	1:D:242:ASP:HB3	2.03	0.41
1:B:365:ALA:HA	1:B:368:GLU:HG2	2.03	0.40
1:A:422:ASN:O	1:A:478:PHE:HA	2.21	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	516/520 (99%)	504 (98%)	12 (2%)	0	100	100
1	B	515/520 (99%)	503 (98%)	12 (2%)	0	100	100
1	C	489/520 (94%)	480 (98%)	9 (2%)	0	100	100
1	D	508/520 (98%)	496 (98%)	12 (2%)	0	100	100
All	All	2028/2080 (98%)	1983 (98%)	45 (2%)	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	474/475 (100%)	458 (97%)	16 (3%)	37	67
1	B	473/475 (100%)	469 (99%)	4 (1%)	81	93
1	C	456/475 (96%)	450 (99%)	6 (1%)	69	88
1	D	469/475 (99%)	460 (98%)	9 (2%)	57	81
All	All	1872/1900 (98%)	1837 (98%)	35 (2%)	57	81

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	14	ASP
1	A	29	GLU
1	A	88	TYR
1	A	122	SER
1	A	131	LEU
1	A	148	ASN
1	A	165	LEU
1	A	241	TYR
1	A	300	GLU
1	A	322	ASN
1	A	370	GLU
1	A	373	LYS
1	A	431	ASN
1	A	467	MET
1	A	485	ASN
1	B	2	ASP
1	B	165	LEU
1	B	241	TYR
1	B	517	LYS
1	C	2	ASP
1	C	148	ASN
1	C	165	LEU
1	C	241	TYR

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Mol	Chain	Res	Type
1	C	347	LYS
1	C	468	SER
1	D	2	ASP
1	D	26	LYS
1	D	29	GLU
1	D	148	ASN
1	D	165	LEU
1	D	241	TYR
1	D	435	ASN
1	D	438	TYR
1	D	485	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	272	GLN
1	A	315	GLN
1	A	349	ASN
1	A	476	ASN
1	A	485	ASN
1	A	499	HIS
1	B	110	GLN
1	B	349	ASN
1	B	476	ASN
1	B	499	HIS
1	B	515	ASN
1	C	56	ASN
1	C	171	ASN
1	C	349	ASN
1	C	476	ASN
1	C	495	ASN
1	D	349	ASN
1	D	435	ASN
1	D	476	ASN
1	D	495	ASN
1	D	499	HIS

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	602	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	B	603	-	4,4,4	0.37	0	6,6,6	0.16	0
2	SO4	C	603	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	B	601	3	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	C	602	3	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	A	601	3	4,4,4	0.35	0	6,6,6	0.18	0
2	SO4	B	604	-	4,4,4	0.34	0	6,6,6	0.15	0
2	SO4	C	601	-	4,4,4	0.43	0	6,6,6	0.16	0
2	SO4	D	601	-	4,4,4	0.41	0	6,6,6	0.26	0
2	SO4	D	602	3	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	B	602	-	4,4,4	0.46	0	6,6,6	0.23	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.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	SO4	1	0
2	C	603	SO4	1	0
2	B	604	SO4	3	0
2	D	601	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	516/520 (99%)	-0.33	6 (1%) 79 78	24, 40, 80, 126	0
1	B	516/520 (99%)	-0.38	6 (1%) 79 78	23, 40, 80, 122	0
1	C	497/520 (95%)	0.01	7 (1%) 75 74	35, 58, 90, 116	0
1	D	512/520 (98%)	-0.08	12 (2%) 60 57	28, 51, 89, 127	0
All	All	2041/2080 (98%)	-0.20	31 (1%) 73 72	23, 48, 86, 127	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	THR	7.4
1	C	298	ASP	3.9
1	D	301	ASP	3.8
1	A	432	THR	3.6
1	C	488	HIS	3.5
1	D	27	ASN	3.3
1	B	368	GLU	3.2
1	B	364	HIS	3.0
1	B	365	ALA	3.0
1	A	429	ASP	2.9
1	A	301	ASP	2.9
1	B	366	LYS	2.7
1	D	56	ASN	2.6
1	D	365	ALA	2.6
1	A	13	ILE	2.5
1	A	433	SER	2.5
1	C	222	PRO	2.4
1	D	489	TYR	2.3
1	A	489	TYR	2.3
1	D	14	ASP	2.2
1	C	440	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	302	GLY	2.2
1	D	297	ASN	2.2
1	C	407	PHE	2.2
1	B	301	ASP	2.1
1	D	22	PHE	2.1
1	C	202	PHE	2.1
1	C	23	LEU	2.0
1	D	47	ASN	2.0
1	D	367	THR	2.0
1	D	492	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 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, 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(Å ²)	Q<0.9
2	SO4	C	603	5/5	0.87	0.28	78,89,103,104	0
2	SO4	B	603	5/5	0.89	0.36	74,75,79,90	0
2	SO4	D	602	5/5	0.90	0.22	101,106,121,126	0
2	SO4	B	604	5/5	0.92	0.22	68,81,93,103	0
3	MG	A	603	1/1	0.93	0.07	29,29,29,29	0
3	MG	B	605	1/1	0.93	0.12	25,25,25,25	0
2	SO4	A	601	5/5	0.95	0.15	69,69,83,94	0
3	MG	C	604	1/1	0.96	0.07	40,40,40,40	0
2	SO4	C	602	5/5	0.97	0.10	64,64,69,70	0
3	MG	D	603	1/1	0.97	0.14	45,45,45,45	0
2	SO4	D	601	5/5	0.98	0.11	51,53,56,56	0
2	SO4	C	601	5/5	0.98	0.09	48,50,53,55	0
2	SO4	B	602	5/5	0.99	0.11	33,33,36,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	602	5/5	0.99	0.09	42,42,45,45	0
2	SO4	B	601	5/5	0.99	0.10	44,47,51,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.