



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:38 AM UTC

PDB ID : 7PJC / pdb_00007pjc
Title : The structure of Candida albicans phosphoglucomutase with isothiazolone modification on Cys359
Authors : Yan, K.; van Aalten, D.M.F.
Deposited on : 2021-08-23
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

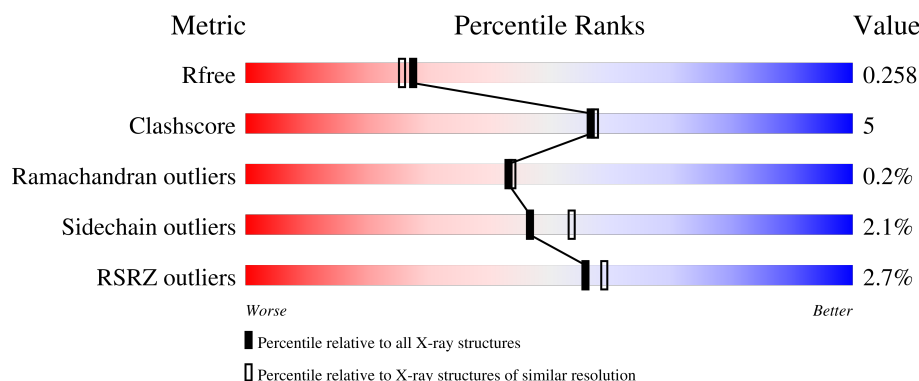
1 Overall quality at a glance

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	565	5% 84% 13%
1	B	565	% 87% 11%

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	A4W	A	602	-	X	-	-

2 Entry composition [i](#)

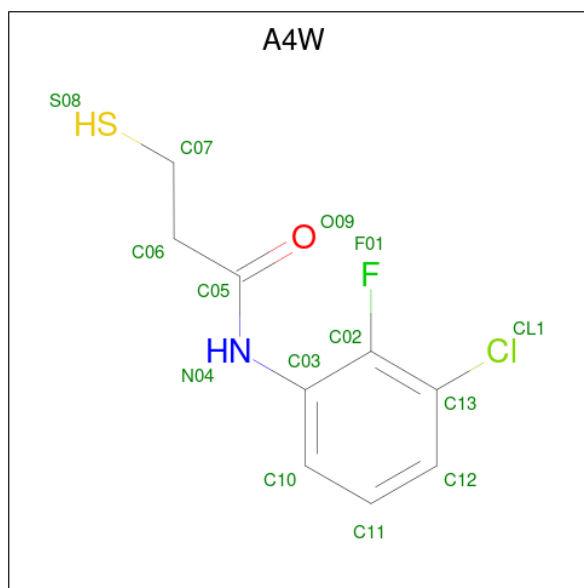
There are 5 unique types of molecules in this entry. The entry contains 9212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoglucomutase.

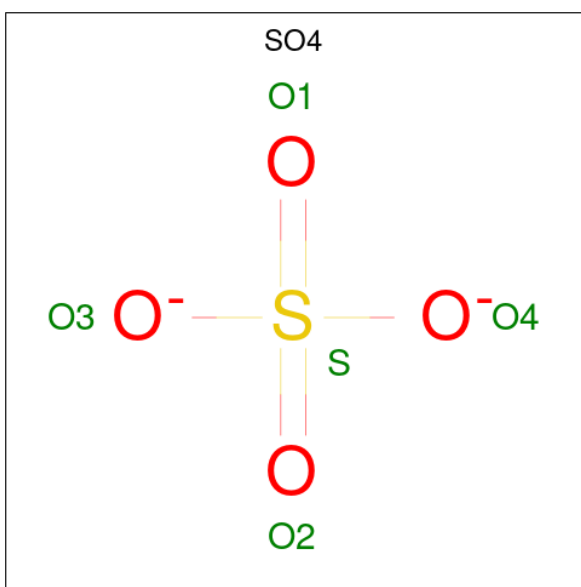
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	553	Total	C	N	O	S	0	3	0
			4301	2753	702	839	7			
1	A	549	Total	C	N	O	S	0	1	0
			4200	2686	684	823	7			

- Molecule 2 is {N}-(3-chloranyl-2-fluoranyl-phenyl)-3-sulfanyl-propanamide (CCD ID: A4W) (formula: C₉H₉ClFNOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	F	N	O	S
			14	9	1	1	1	1	1
2	A	1	Total	C	Cl	F	N	O	S
			14	9	1	1	1	1	1

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

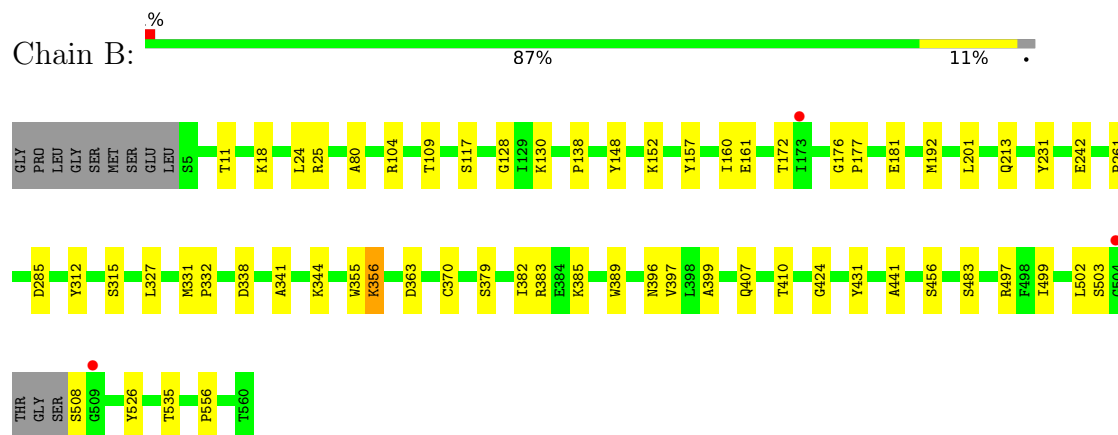
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	385	Total	O	0	0
			385	385		
5	A	242	Total	O	0	0
			242	242		

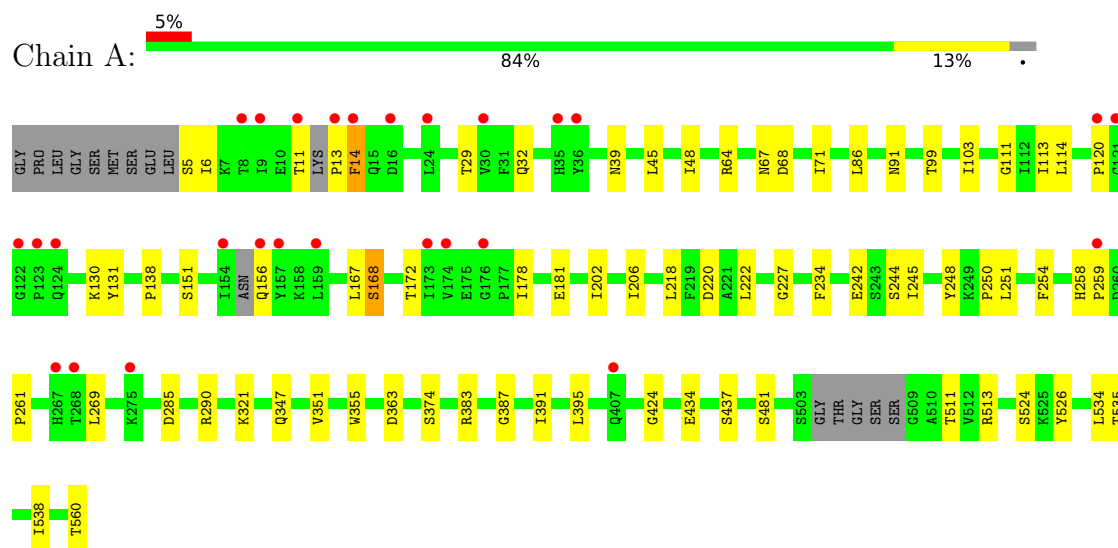
3 Residue-property plots [i](#)

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: Phosphoglucumutase



• Molecule 1: Phosphoglucumutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.74Å 86.44Å 110.15Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	67.97 – 2.11 67.97 – 2.11	Depositor EDS
% Data completeness (in resolution range)	66.3 (67.97-2.11) 66.3 (67.97-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.255 0.191 , 0.258	Depositor DCC
R_{free} test set	2324 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9212	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2757e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, A4W

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	0.33	0/4290	0.51	0/5821
1	B	0.37	0/4402	0.54	0/5969
All	All	0.35	0/8692	0.52	0/11790

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4200	0	4025	40	0
1	B	4301	0	4195	39	0
2	A	14	0	0	0	0
2	B	14	0	0	1	0
3	A	20	0	0	1	0
3	B	30	0	0	0	0
4	A	6	0	8	0	0
5	A	242	0	0	3	0
5	B	385	0	0	6	0
All	All	9212	0	8228	78	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 5.

All (78) 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:363:ASP:OD1	1:A:383:ARG:NH2	2.07	0.86
1:A:13:PRO:HD2	1:A:39:ASN:HD21	1.55	0.71
1:B:431:TYR:HB3	1:B:556:PRO:HB3	1.73	0.71
1:B:172:THR:HG22	1:B:181:GLU:HG3	1.74	0.70
1:B:363:ASP:OD1	1:B:383:ARG:NH2	2.23	0.68
1:A:321:LYS:NZ	5:A:703:HOH:O	2.27	0.68
1:B:11:THR:HG21	1:B:157:TYR:HE1	1.60	0.67
1:A:218:LEU:HD23	1:A:269:LEU:HD12	1.79	0.65
1:A:71:ILE:HG21	1:A:167:LEU:HD11	1.80	0.62
1:B:213:GLN:NE2	1:B:410:THR:H	1.97	0.62
1:B:213:GLN:HE22	1:B:410:THR:H	1.48	0.60
1:A:86:LEU:HG	1:A:178:ILE:HD11	1.83	0.60
1:B:148:TYR:CZ	1:B:152:LYS:HD2	2.39	0.57
1:A:68:ASP:HA	1:A:71:ILE:HD12	1.87	0.56
1:A:29:THR:HA	1:A:32:GLN:HB2	1.87	0.55
1:A:434:GLU:HA	1:A:511:THR:HG23	1.89	0.54
1:B:25:ARG:NH2	1:B:117[B]:SER:OG	2.41	0.54
1:B:456:SER:HB3	1:A:481:SER:HB2	1.90	0.54
1:A:254:PHE:CD2	1:A:259:PRO:HG3	2.42	0.54
1:B:535:THR:HG23	5:B:759:HOH:O	2.07	0.54
1:A:234:PHE:HE1	1:A:395:LEU:HD11	1.74	0.53
1:A:513:ARG:NE	3:A:603:SO4:O3	2.34	0.53
1:B:327:LEU:HD12	1:B:341:ALA:HB2	1.91	0.53
1:A:172:THR:HG22	1:A:181:GLU:HG3	1.91	0.52
1:A:202:ILE:O	1:A:206:ILE:HD12	2.10	0.51
1:B:231:TYR:OH	1:B:242:GLU:OE2	2.20	0.51
1:A:534:LEU:O	1:A:538:ILE:HG13	2.12	0.50
1:B:385:LYS:NZ	5:B:705:HOH:O	2.44	0.50
1:A:220:ASP:OD1	1:A:222:LEU:HD23	2.11	0.49
1:B:138:PRO:HB2	1:B:355:TRP:CZ2	2.47	0.49
1:A:103:ILE:HD11	1:A:111:GLY:HA3	1.94	0.49
1:A:11:THR:OG1	1:A:156:GLN:HA	2.12	0.48
1:B:407:GLN:H	1:B:407:GLN:CD	2.21	0.48
1:A:285:ASP:CG	1:A:290:ARG:HB2	2.38	0.48
1:B:192:MET:HE2	1:B:192:MET:HB3	1.73	0.48
1:A:424:GLY:HA2	1:A:526:TYR:OH	2.13	0.48
1:A:245:ILE:HG12	1:A:248:TYR:HD2	1.78	0.48
1:A:387:GLY:O	1:A:391:ILE:HG13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LYS:HG3	1:B:148:TYR:CD2	2.50	0.47
1:B:261:PRO:HD3	1:B:285:ASP:HB3	1.97	0.46
1:A:91:ASN:OD1	1:A:168:SER:HA	2.16	0.45
1:A:250:PRO:O	1:A:251:LEU:HD23	2.17	0.45
1:A:560:THR:HG22	5:A:739:HOH:O	2.16	0.45
1:A:11:THR:HB	1:A:13:PRO:HG2	1.98	0.45
1:B:379:SER:HB3	1:B:389:TRP:CZ2	2.52	0.45
1:B:11:THR:HG21	1:B:157:TYR:CE1	2.48	0.44
1:A:261:PRO:HD3	1:A:285:ASP:HB3	1.98	0.44
1:B:312:TYR:HB2	1:B:397:VAL:HG22	1.99	0.44
1:B:24:LEU:O	1:B:128:GLY:HA2	2.18	0.43
1:B:104:ARG:HH12	1:B:383:ARG:HG3	1.83	0.43
1:B:130:LYS:HB2	5:B:879:HOH:O	2.18	0.43
1:A:64:ARG:HG2	1:A:67:ASN:ND2	2.33	0.43
1:B:356:LYS:HB3	5:B:935:HOH:O	2.18	0.43
1:B:441:ALA:HB1	1:B:502:LEU:HD21	2.01	0.43
1:A:5:SER:OG	1:A:6:ILE:N	2.48	0.43
1:B:338:ASP:OD2	1:B:338:ASP:N	2.50	0.43
1:B:497:ARG:CZ	1:B:499:ILE:HD11	2.49	0.42
1:B:148:TYR:CE1	1:B:152:LYS:HD2	2.55	0.42
1:B:201:LEU:HG	1:B:399:ALA:HB1	2.02	0.42
1:A:120:PRO:HG3	1:A:258:HIS:NE2	2.35	0.42
1:B:104:ARG:HD3	5:B:828:HOH:O	2.20	0.42
1:A:48:ILE:HG12	1:A:131:TYR:CZ	2.56	0.41
1:B:407:GLN:H	1:B:407:GLN:NE2	2.19	0.41
1:A:45:LEU:HA	1:A:48:ILE:HD12	2.02	0.41
1:A:13:PRO:HB2	1:A:14:PHE:H	1.50	0.41
1:B:331:MET:HE3	1:B:331:MET:HB3	1.90	0.41
1:A:172:THR:CG2	1:A:181:GLU:HG3	2.50	0.41
1:B:344:LYS:HE3	5:B:866:HOH:O	2.20	0.41
1:B:80:ALA:HB2	1:B:160:ILE:HG13	2.02	0.41
1:A:138:PRO:HB2	1:A:355:TRP:CZ2	2.56	0.41
1:A:227:GLY:HA3	1:A:248:TYR:O	2.21	0.41
1:B:370:CYS:SG	2:B:601:A4W:C12	3.10	0.40
1:B:424:GLY:HA2	1:B:526:TYR:OH	2.21	0.40
1:A:99:THR:HG21	1:A:113:ILE:HG12	2.02	0.40
1:B:176:GLY:HA3	1:B:177:PRO:HD3	1.91	0.40
1:B:331:MET:HB3	1:B:332:PRO:HD3	2.04	0.40
1:A:347:GLN:NE2	5:A:728:HOH:O	2.54	0.40
1:A:513:ARG:HG2	1:A:513:ARG:HH11	1.86	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	542/565 (96%)	519 (96%)	21 (4%)	2 (0%)	30	28
1	B	552/565 (98%)	532 (96%)	20 (4%)	0	100	100
All	All	1094/1130 (97%)	1051 (96%)	41 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	SER
1	A	14	PHE

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	440/483 (91%)	430 (98%)	10 (2%)	44	50
1	B	463/483 (96%)	454 (98%)	9 (2%)	50	57
All	All	903/966 (94%)	884 (98%)	19 (2%)	47	54

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	109	THR
1	B	161	GLU
1	B	315	SER
1	B	356	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	382	ILE
1	B	396	ASN
1	B	483	SER
1	B	503	SER
1	B	508	SER
1	A	114	LEU
1	A	130	LYS
1	A	151	SER
1	A	168	SER
1	A	242	GLU
1	A	351	VAL
1	A	374	SER
1	A	437	SER
1	A	524	SER
1	A	535	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	GLN
1	B	53	GLN
1	B	119	ASN
1	B	124	GLN
1	B	213	GLN
1	B	277	ASN
1	B	291	ASN
1	B	404	GLN
1	B	405	ASN
1	B	407	GLN
1	B	416	GLN
1	A	39	ASN
1	A	145	ASN
1	A	236	ASN
1	A	247	ASN
1	A	347	GLN
1	A	396	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	SO4	B	603	-	4,4,4	0.34	0	6,6,6	0.35	0
3	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.44	0
3	SO4	B	602	-	4,4,4	0.28	0	6,6,6	0.12	0
4	GOL	A	601	-	5,5,5	1.46	1 (20%)	5,5,5	1.26	1 (20%)
3	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.25	0
3	SO4	B	607	-	4,4,4	0.28	0	6,6,6	0.20	0
3	SO4	B	606	-	4,4,4	0.28	0	6,6,6	0.10	0
3	SO4	A	605	-	4,4,4	0.25	0	6,6,6	0.23	0
2	A4W	B	601	1	13,14,14	1.94	6 (46%)	17,18,18	1.68	3 (17%)
3	SO4	A	606	-	4,4,4	0.26	0	6,6,6	0.20	0
3	SO4	B	605	-	4,4,4	0.23	0	6,6,6	0.25	0
2	A4W	A	602	1	13,14,14	2.06	8 (61%)	17,18,18	2.07	4 (23%)
3	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.18	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
2	A4W	B	601	1	-	3/7/7/7	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A4W	A	602	1	-	4/7/7/7	0/1/1/1
4	GOL	A	601	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	A4W	C05-N04	3.63	1.43	1.35
2	B	601	A4W	F01-C02	-2.65	1.31	1.34
2	B	601	A4W	C13-C02	2.62	1.43	1.38
2	B	601	A4W	C07-S08	-2.53	1.70	1.80
2	A	602	A4W	F01-C02	-2.46	1.31	1.34
2	A	602	A4W	C11-C12	2.44	1.43	1.38
2	B	601	A4W	C05-N04	2.39	1.40	1.35
4	A	601	GOL	C3-C2	2.35	1.60	1.51
2	A	602	A4W	C13-C02	2.27	1.42	1.38
2	A	602	A4W	C03-C02	2.22	1.42	1.38
2	A	602	A4W	C11-C10	2.16	1.42	1.38
2	A	602	A4W	C07-S08	-2.10	1.71	1.80
2	B	601	A4W	C11-C12	2.05	1.42	1.38
2	A	602	A4W	O09-C05	-2.03	1.19	1.23
2	B	601	A4W	O09-C05	-2.02	1.19	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	A4W	C12-C13-C02	5.16	122.41	119.37
2	B	601	A4W	C12-C13-C02	3.93	121.69	119.37
2	A	602	A4W	C02-C13-CL1	-3.82	117.00	119.44
2	B	601	A4W	C10-C03-N04	3.05	128.88	121.82
2	A	602	A4W	C07-C06-C05	2.69	118.94	112.80
2	A	602	A4W	C10-C03-N04	2.68	128.03	121.82
2	B	601	A4W	F01-C02-C13	2.58	122.92	119.14
4	A	601	GOL	C3-C2-C1	-2.34	103.23	111.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	A4W	C05-C06-C07-S08
2	A	602	A4W	C05-C06-C07-S08
4	A	601	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
2	B	601	A4W	O09-C05-N04-C03
2	A	602	A4W	O09-C05-N04-C03
2	B	601	A4W	C06-C05-N04-C03
2	A	602	A4W	C06-C05-N04-C03
2	A	602	A4W	C02-C03-N04-C05

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	SO4	1	0
2	B	601	A4W	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, 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	549/565 (97%)	0.24	27 (4%) 35 37	13, 36, 65, 97	1 (0%)
1	B	553/565 (97%)	-0.30	3 (0%) 87 89	11, 24, 40, 62	3 (0%)
All	All	1102/1130 (97%)	-0.03	30 (2%) 56 59	11, 28, 59, 97	4 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	GLY	5.0
1	A	14	PHE	4.5
1	A	156	GLN	3.9
1	A	122	GLY	3.3
1	A	123	PRO	3.3
1	B	509	GLY	3.2
1	A	13	PRO	3.2
1	A	157	TYR	3.0
1	A	124	GLN	3.0
1	A	407	GLN	2.8
1	A	30	VAL	2.7
1	A	11	THR	2.7
1	A	120	PRO	2.6
1	A	8	THR	2.5
1	A	174	VAL	2.5
1	A	173	ILE	2.5
1	A	36	TYR	2.4
1	A	121	GLY	2.4
1	A	9	ILE	2.4
1	A	154	ILE	2.4
1	A	24	LEU	2.3
1	A	267	HIS	2.3
1	A	275	LYS	2.3
1	A	16	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	173	ILE	2.2
1	A	176	GLY	2.2
1	A	268	THR	2.2
1	A	35	HIS	2.1
1	A	159	LEU	2.1
1	A	259	PRO	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(Å ²)	Q<0.9
3	SO4	A	604	5/5	0.70	0.15	82,90,99,110	0
3	SO4	A	605	5/5	0.71	0.14	84,87,97,103	0
3	SO4	B	605	5/5	0.72	0.16	83,85,98,102	0
3	SO4	A	606	5/5	0.75	0.13	73,73,86,91	0
3	SO4	B	607	5/5	0.82	0.13	64,65,73,85	0
3	SO4	B	604	5/5	0.82	0.16	74,75,90,93	0
3	SO4	A	603	5/5	0.85	0.13	41,47,56,60	0
4	GOL	A	601	6/6	0.88	0.15	21,29,43,47	0
3	SO4	B	606	5/5	0.91	0.08	58,63,68,72	0
3	SO4	B	603	5/5	0.93	0.14	46,48,51,58	0
2	A4W	B	601	14/14	0.94	0.08	20,24,32,38	0
3	SO4	B	602	5/5	0.94	0.10	48,48,55,57	0
2	A4W	A	602	14/14	0.96	0.07	22,27,41,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.