



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2024 – 12:06 PM EDT

PDB ID : 2HZK  
Title : Crystal structures of a sodium-alpha-keto acid binding subunit from a TRAP transporter in its open form  
Authors : Gonin, S.; Arnoux, P.; Pierru, B.; Alonso, B.; Sabaty, M.; Pignol, D.  
Deposited on : 2006-08-09  
Resolution : 1.70 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](mailto: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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

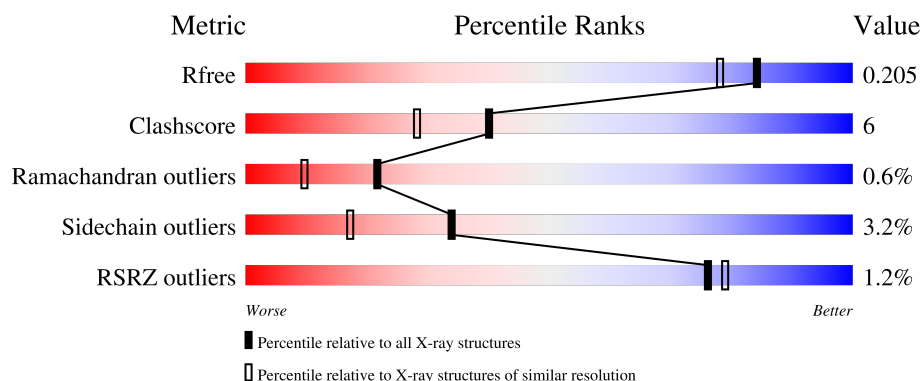
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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  $\geq 3$ , 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	365	<div> <div>2%</div> <div>80% 10% 8%</div> </div>
1	B	365	<div> <div>83% 8% 8%</div> </div>
1	C	365	<div> <div>2%</div> <div>78% 12% 8%</div> </div>
1	D	365	<div> <div>2%</div> <div>79% 13% 7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11298 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 TRAP-T family sorbitol/mannitol transporter, periplasmic binding protein, SmoM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	Se	0	3	0
			2637	1701	432	490	4	10			
1	B	336	Total	C	N	O	S	Se	0	1	0
			2634	1700	432	488	4	10			
1	C	335	Total	C	N	O	S	Se	0	0	0
			2624	1693	431	486	4	10			
1	D	338	Total	C	N	O	S	Se	0	1	0
			2648	1708	435	491	4	10			

There are 40 discrepancies between the modelled and reference sequences:

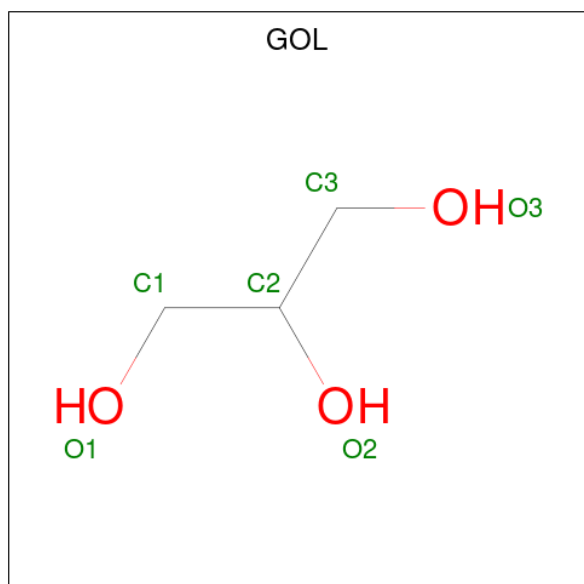
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MSE	MET	modified residue	UNP Q3J1R2
A	157	MSE	MET	modified residue	UNP Q3J1R2
A	171	MSE	MET	modified residue	UNP Q3J1R2
A	176	MSE	MET	modified residue	UNP Q3J1R2
A	186	MSE	MET	modified residue	UNP Q3J1R2
A	248	MSE	MET	modified residue	UNP Q3J1R2
A	276	MSE	MET	modified residue	UNP Q3J1R2
A	320	MSE	MET	modified residue	UNP Q3J1R2
A	356	MSE	MET	modified residue	UNP Q3J1R2
A	357	MSE	MET	modified residue	UNP Q3J1R2
B	57	MSE	MET	modified residue	UNP Q3J1R2
B	157	MSE	MET	modified residue	UNP Q3J1R2
B	171	MSE	MET	modified residue	UNP Q3J1R2
B	176	MSE	MET	modified residue	UNP Q3J1R2
B	186	MSE	MET	modified residue	UNP Q3J1R2
B	248	MSE	MET	modified residue	UNP Q3J1R2
B	276	MSE	MET	modified residue	UNP Q3J1R2
B	320	MSE	MET	modified residue	UNP Q3J1R2
B	356	MSE	MET	modified residue	UNP Q3J1R2
B	357	MSE	MET	modified residue	UNP Q3J1R2

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	57	MSE	MET	modified residue	UNP Q3J1R2
C	157	MSE	MET	modified residue	UNP Q3J1R2
C	171	MSE	MET	modified residue	UNP Q3J1R2
C	176	MSE	MET	modified residue	UNP Q3J1R2
C	186	MSE	MET	modified residue	UNP Q3J1R2
C	248	MSE	MET	modified residue	UNP Q3J1R2
C	276	MSE	MET	modified residue	UNP Q3J1R2
C	320	MSE	MET	modified residue	UNP Q3J1R2
C	356	MSE	MET	modified residue	UNP Q3J1R2
C	357	MSE	MET	modified residue	UNP Q3J1R2
D	57	MSE	MET	modified residue	UNP Q3J1R2
D	157	MSE	MET	modified residue	UNP Q3J1R2
D	171	MSE	MET	modified residue	UNP Q3J1R2
D	176	MSE	MET	modified residue	UNP Q3J1R2
D	186	MSE	MET	modified residue	UNP Q3J1R2
D	248	MSE	MET	modified residue	UNP Q3J1R2
D	276	MSE	MET	modified residue	UNP Q3J1R2
D	320	MSE	MET	modified residue	UNP Q3J1R2
D	356	MSE	MET	modified residue	UNP Q3J1R2
D	357	MSE	MET	modified residue	UNP Q3J1R2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

Continued on next page...

*Continued from previous page...*

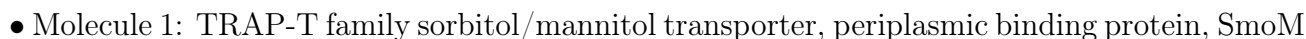
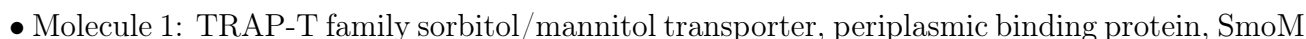
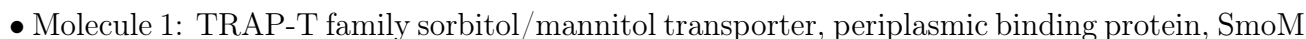
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

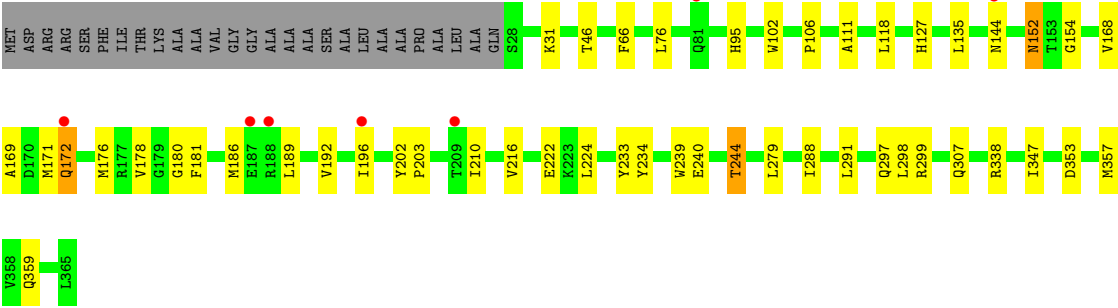
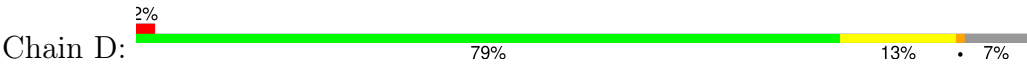
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		
3	B	201	Total	O	0	0
			201	201		
3	C	178	Total	O	0	0
			178	178		
3	D	149	Total	O	0	0
			149	149		



- Molecule 1: TRAP-T family sorbitol/mannitol transporter, periplasmic binding protein, SmoM





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.50Å 63.83Å 127.90Å 90.00° 106.58° 90.00°	Depositor
Resolution (Å)	60.00 – 1.70 60.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (60.00-1.70) 98.5 (60.00-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.206 0.178 , 0.205	Depositor DCC
$R_{free}$ test set	8721 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL

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	0.62	0/2709	0.63	0/3667
1	B	0.63	0/2707	0.63	1/3663 (0.0%)
1	C	0.59	0/2693	0.63	1/3644 (0.0%)
1	D	0.59	0/2718	0.61	0/3680
All	All	0.61	0/10827	0.63	2/14654 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	GLU	CA-CB-CG	7.24	129.32	113.40
1	B	191	VAL	CG1-CB-CG2	5.32	119.42	110.90

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	2637	0	2511	38	0
1	B	2634	0	2516	24	0
1	C	2624	0	2503	46	0
1	D	2648	0	2523	35	0
2	A	6	0	8	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	203	0	0	4	0
3	B	201	0	0	5	0
3	C	178	0	0	6	0
3	D	149	0	0	4	0
All	All	11298	0	10085	134	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 6.

All (134) 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:127:HIS:HE1	1:A:244:THR:HG21	1.09	1.15
1:D:127:HIS:HE1	1:D:244[B]:THR:HG21	1.12	1.14
1:D:127:HIS:HE1	1:D:244[A]:THR:HG21	0.97	1.13
1:B:168:VAL:HA	1:B:171:MSE:HE3	1.23	1.12
1:D:127:HIS:CE1	1:D:244[A]:THR:HG21	1.87	1.09
1:C:127:HIS:HE1	1:C:244:THR:HG21	1.16	1.08
1:B:168:VAL:HA	1:B:171:MSE:CE	1.87	1.04
1:A:127:HIS:CE1	1:A:244:THR:HG21	1.93	1.03
1:D:127:HIS:CE1	1:D:244[B]:THR:HG21	1.97	0.99
1:C:127:HIS:CE1	1:C:244:THR:HG21	1.99	0.97
1:B:171:MSE:HE2	1:B:305:ILE:HG12	1.47	0.95
1:A:307:GLN:HE22	1:B:359:GLN:HE22	1.07	0.94
1:D:244[B]:THR:HG22	3:D:811:HOH:O	1.71	0.90
1:A:127:HIS:HE1	1:A:244:THR:CG2	1.85	0.88
1:C:219:TYR:HE1	3:C:953:HOH:O	1.56	0.86
1:B:168:VAL:CA	1:B:171:MSE:HE3	2.07	0.84
1:C:307:GLN:HE22	1:D:359:GLN:HE22	1.26	0.84
1:C:168:VAL:HA	1:C:171:MSE:HE2	1.59	0.83
1:C:307:GLN:HE22	1:D:359:GLN:NE2	1.77	0.82
1:C:127:HIS:HE1	1:C:244:THR:CG2	1.93	0.80
1:D:152:ASN:HD22	1:D:154:GLY:H	1.29	0.80
1:D:127:HIS:HE1	1:D:244[A]:THR:CG2	1.89	0.78
1:C:152:ASN:HD22	1:C:154:GLY:H	1.29	0.77
1:B:152:ASN:HD22	1:B:154:GLY:H	1.32	0.77
1:A:32:VAL:N	3:A:961:HOH:O	2.17	0.77
1:B:168:VAL:HG23	1:B:304:GLU:HG2	1.66	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASN:HB3	3:D:850:HOH:O	1.87	0.74
1:A:152:ASN:HD22	1:A:154:GLY:H	1.35	0.74
1:C:34:TRP:CG	1:C:92:GLU:HG2	2.23	0.73
1:D:168:VAL:HA	1:D:171:MSE:HE2	1.69	0.73
1:D:196:ILE:HD11	1:D:210:ILE:HG21	1.72	0.71
1:C:34:TRP:CD1	1:C:92:GLU:HG2	2.26	0.71
1:A:307:GLN:NE2	1:B:359:GLN:HE22	1.87	0.70
1:A:279:LEU:HD22	1:A:283:LYS:HE2	1.72	0.70
1:A:34:TRP:HB3	1:A:92[A]:GLU:HG3	1.73	0.69
1:C:279:LEU:HD11	1:C:283:LYS:HE2	1.76	0.67
1:A:168:VAL:HG13	1:A:171:MSE:HE2	1.76	0.67
1:A:34:TRP:CB	1:A:92[A]:GLU:HG3	2.26	0.66
1:A:90:THR:HG22	1:D:180:GLY:H	1.62	0.65
1:C:168:VAL:HG13	1:C:171:MSE:CE	2.28	0.64
1:D:176:MSE:SE	1:D:186:MSE:HE1	2.48	0.64
1:A:359:GLN:HE22	1:B:307:GLN:HE22	1.44	0.64
1:C:219:TYR:CE1	3:C:953:HOH:O	2.39	0.64
1:D:169:ALA:O	1:D:172:GLN:HG3	2.01	0.61
1:D:239:TRP:CD1	1:D:240:GLU:HG2	2.36	0.60
1:C:222:GLU:HG3	1:C:291:LEU:HD13	1.83	0.60
1:C:31:LYS:HG2	1:C:65:ASN:HD21	1.68	0.58
1:D:244[A]:THR:HB	3:D:811:HOH:O	2.03	0.57
1:C:46:THR:HG23	1:C:279:LEU:HD23	1.85	0.57
1:C:202:TYR:HB3	1:C:203:PRO:HD3	1.87	0.56
1:B:95:HIS:HD2	3:B:804:HOH:O	1.87	0.56
1:D:171:MSE:HE1	1:D:189:LEU:HD13	1.87	0.56
1:A:171:MSE:CE	1:A:189:LEU:HB3	2.37	0.55
1:C:168:VAL:HG23	1:C:304:GLU:HG2	1.87	0.55
1:A:90:THR:HG22	1:D:180:GLY:N	2.22	0.55
1:C:31:LYS:HG2	1:C:65:ASN:ND2	2.22	0.55
1:A:34:TRP:CG	1:A:92[A]:GLU:HG3	2.42	0.54
1:B:304:GLU:HG3	3:B:917:HOH:O	2.07	0.54
1:C:196:ILE:HD11	1:C:210:ILE:HG21	1.88	0.54
1:B:365:LEU:OXT	3:B:976:HOH:O	2.18	0.54
1:D:46:THR:HG23	1:D:279:LEU:HD23	1.89	0.54
1:C:168:VAL:HG13	1:C:171:MSE:HE2	1.89	0.54
1:B:168:VAL:HA	1:B:171:MSE:HE2	1.86	0.53
1:B:127:HIS:HE1	1:B:244:THR:OG1	1.92	0.53
1:B:118:LEU:HD21	1:B:338:ARG:HA	1.91	0.53
1:A:307:GLN:HE22	1:B:359:GLN:NE2	1.91	0.52
1:D:178:VAL:HG11	1:D:186:MSE:HE3	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:GLU:HB3	1:C:243:PRO:HG3	1.91	0.52
1:D:222:GLU:HA	1:D:291:LEU:HD21	1.91	0.52
1:C:168:VAL:CA	1:C:171:MSE:HE2	2.35	0.51
1:C:307:GLN:HG3	3:C:972:HOH:O	2.09	0.51
1:A:118:LEU:HD21	1:A:338:ARG:HA	1.91	0.51
1:C:288:ILE:HD11	1:C:298:LEU:HD21	1.91	0.51
1:D:288:ILE:HD11	1:D:298:LEU:HD21	1.93	0.51
1:C:171:MSE:HE3	1:C:189:LEU:HB3	1.93	0.51
1:B:174:LEU:HB3	1:B:191:VAL:HB	1.91	0.51
1:D:111:ALA:O	1:D:244[B]:THR:OG1	2.28	0.50
1:C:88:GLU:HG3	1:C:90:THR:HG23	1.93	0.50
1:C:88:GLU:OE2	1:C:90:THR:HG21	2.11	0.50
1:D:95:HIS:HD2	3:D:805:HOH:O	1.95	0.49
1:C:171:MSE:HE1	1:C:189:LEU:HD13	1.94	0.49
1:A:95:HIS:HD2	3:A:802:HOH:O	1.93	0.49
1:D:102:TRP:CZ3	1:D:106:PRO:HB3	2.48	0.49
1:A:234:TYR:HA	1:A:299:ARG:O	2.13	0.48
1:D:196:ILE:CD1	1:D:210:ILE:HG21	2.40	0.48
1:A:171:MSE:HE1	1:A:189:LEU:HB3	1.96	0.48
1:B:219:TYR:HE1	3:B:926:HOH:O	1.96	0.48
1:D:202:TYR:HB3	1:D:203:PRO:HD3	1.96	0.48
1:A:168:VAL:HG13	1:A:171:MSE:CE	2.43	0.47
1:A:288:ILE:HD11	1:A:298:LEU:HD21	1.95	0.47
1:C:34:TRP:CD1	1:C:92:GLU:CG	2.96	0.47
1:C:359:GLN:OE1	1:C:364:LYS:HD2	2.15	0.47
1:B:234:TYR:HA	1:B:299:ARG:O	2.15	0.47
1:C:95:HIS:HD2	3:C:808:HOH:O	1.97	0.46
1:C:359:GLN:HE22	1:D:307:GLN:HE22	1.64	0.46
1:B:288:ILE:HD11	1:B:298:LEU:HD21	1.98	0.46
1:A:44:LEU:HD21	2:A:801:GOL:H12	1.97	0.46
1:C:88:GLU:OE2	1:C:90:THR:CG2	2.64	0.46
1:C:163:ARG:NH1	3:C:915:HOH:O	2.48	0.45
1:A:240:GLU:HB3	1:A:243:PRO:HG3	1.99	0.45
1:A:168:VAL:HA	1:A:171:MSE:HE2	1.99	0.45
1:D:152:ASN:ND2	1:D:154:GLY:H	2.06	0.45
1:A:331:TRP:CD1	1:A:335:LYS:HE2	2.52	0.44
1:D:297:GLN:HG3	1:D:299:ARG:NH2	2.32	0.44
1:C:97:VAL:HG11	1:C:99:TYR:CZ	2.53	0.44
1:C:152:ASN:ND2	1:C:154:GLY:H	2.07	0.44
1:A:186:MSE:HB3	1:A:191[B]:VAL:HG13	2.00	0.44
1:B:152:ASN:ND2	1:B:154:GLY:H	2.10	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ILE:HD11	1:B:210:ILE:HG21	2.00	0.43
1:D:234:TYR:HA	1:D:299:ARG:O	2.17	0.43
1:B:162:ARG:NH1	3:B:911:HOH:O	2.52	0.43
1:D:118:LEU:HD21	1:D:338:ARG:HA	2.01	0.43
1:A:350:TYR:O	1:A:354:THR:HG23	2.19	0.43
1:C:168:VAL:HG23	1:C:304:GLU:CG	2.49	0.42
1:A:152:ASN:ND2	1:A:154:GLY:H	2.09	0.42
1:A:127:HIS:HD2	3:A:831:HOH:O	2.02	0.42
1:A:171:MSE:HE1	1:A:189:LEU:HD13	2.01	0.42
1:C:127:HIS:HD2	3:C:815:HOH:O	2.03	0.42
1:C:102:TRP:CE2	1:C:180:GLY:HA2	2.55	0.42
1:A:90:THR:HG21	3:A:943:HOH:O	2.19	0.41
1:A:95:HIS:HE1	1:A:150:GLY:O	2.03	0.41
1:C:97:VAL:HG11	1:C:99:TYR:CE2	2.54	0.41
1:C:233:TYR:HB3	1:C:298:LEU:HD23	2.01	0.41
1:C:346:GLN:HA	1:C:350:TYR:HB2	2.02	0.41
1:A:186:MSE:HB3	1:A:191[B]:VAL:CG1	2.51	0.41
1:C:56:LYS:HE2	1:C:60:GLU:OE2	2.21	0.41
1:B:196:ILE:CD1	1:B:210:ILE:HG21	2.50	0.41
1:D:178:VAL:HG21	1:D:186:MSE:CE	2.51	0.41
1:A:202:TYR:HB3	1:A:203:PRO:HD3	2.03	0.40
1:C:234:TYR:HA	1:C:299:ARG:O	2.22	0.40
1:D:353:ASP:HB3	1:D:357:MSE:HE3	2.02	0.40
1:C:196:ILE:CD1	1:C:210:ILE:HG21	2.52	0.40
1:A:171:MSE:HE3	1:A:189:LEU:HB3	2.04	0.40
1:A:174:LEU:HB3	1:A:191[B]:VAL:HB	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	335/365 (92%)	324 (97%)	9 (3%)	2 (1%)	22	10
1	B	335/365 (92%)	324 (97%)	9 (3%)	2 (1%)	22	10
1	C	333/365 (91%)	324 (97%)	7 (2%)	2 (1%)	22	10
1	D	337/365 (92%)	327 (97%)	8 (2%)	2 (1%)	22	10
All	All	1340/1460 (92%)	1299 (97%)	33 (2%)	8 (1%)	22	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	347	ILE
1	A	216	VAL
1	C	216	VAL
1	D	216	VAL
1	D	347	ILE
1	A	347	ILE
1	B	347	ILE
1	B	216	VAL

### 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	267/272 (98%)	260 (97%)	7 (3%)	41	24
1	B	267/272 (98%)	260 (97%)	7 (3%)	41	24
1	C	265/272 (97%)	256 (97%)	9 (3%)	32	15
1	D	267/272 (98%)	255 (96%)	12 (4%)	23	9
All	All	1066/1088 (98%)	1031 (97%)	35 (3%)	34	16

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

Mol	Chain	Res	Type
1	A	66	PHE
1	A	90	THR
1	A	135	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	152	ASN
1	A	192	VAL
1	A	244	THR
1	A	291	LEU
1	B	66	PHE
1	B	76	LEU
1	B	97	VAL
1	B	135	LEU
1	B	152	ASN
1	B	192	VAL
1	B	224	LEU
1	C	31	LYS
1	C	66	PHE
1	C	76	LEU
1	C	92	GLU
1	C	135	LEU
1	C	152	ASN
1	C	192	VAL
1	C	244	THR
1	C	291	LEU
1	D	31	LYS
1	D	66	PHE
1	D	76	LEU
1	D	135	LEU
1	D	152	ASN
1	D	172	GLN
1	D	181	PHE
1	D	192	VAL
1	D	224	LEU
1	D	233	TYR
1	D	244[A]	THR
1	D	244[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	127	HIS
1	A	152	ASN
1	A	275	ASN
1	B	67	GLN
1	B	69	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	95	HIS
1	B	127	HIS
1	B	152	ASN
1	B	194	GLN
1	B	275	ASN
1	B	278	GLN
1	B	307	GLN
1	B	359	GLN
1	C	65	ASN
1	C	95	HIS
1	C	127	HIS
1	C	152	ASN
1	C	275	ASN
1	D	95	HIS
1	D	127	HIS
1	D	152	ASN
1	D	195	GLN
1	D	275	ASN
1	D	278	GLN
1	D	307	GLN
1	D	359	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](#)

4 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	GOL	C	803	-	5,5,5	0.36	0	5,5,5	0.39	0
2	GOL	B	802	-	5,5,5	0.35	0	5,5,5	0.45	0
2	GOL	A	801	-	5,5,5	0.40	0	5,5,5	0.61	0
2	GOL	D	804	-	5,5,5	0.32	0	5,5,5	0.40	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	GOL	C	803	-	-	0/4/4/4	-
2	GOL	B	802	-	-	1/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	D	804	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	C1-C2-C3-O3
2	B	802	GOL	C1-C2-C3-O3
2	D	804	GOL	C1-C2-C3-O3
2	A	801	GOL	O2-C2-C3-O3
2	D	804	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	324/365 (88%)	-0.32	3 (0%) 81 83	5, 14, 24, 31	3 (0%)
1	B	326/365 (89%)	-0.31	0 100 100	7, 14, 24, 31	1 (0%)
1	C	325/365 (89%)	-0.10	5 (1%) 71 74	9, 16, 30, 37	0
1	D	328/365 (89%)	0.00	7 (2%) 63 66	5, 17, 33, 39	1 (0%)
All	All	1303/1460 (89%)	-0.18	15 (1%) 76 79	5, 15, 29, 39	5 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	172	GLN	3.9
1	C	163	ARG	3.2
1	D	196	ILE	2.4
1	A	322	ALA	2.4
1	C	350	TYR	2.4
1	D	209	THR	2.2
1	C	181	PHE	2.1
1	D	144	ASN	2.1
1	C	90	THR	2.1
1	D	188	ARG	2.1
1	A	315	GLU	2.1
1	D	187	GLU	2.1
1	D	81	GLN	2.0
1	C	209	THR	2.0
1	A	65	ASN	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<sup>th</sup> 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	GOL	C	803	6/6	0.83	0.18	41,43,44,46	0
2	GOL	B	802	6/6	0.85	0.15	37,38,39,42	0
2	GOL	A	801	6/6	0.87	0.13	32,33,33,33	0
2	GOL	D	804	6/6	0.93	0.09	27,30,31,31	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.