



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:56 AM GMT

PDB ID : 3C6Q
Title : Apo and ligand-bound form of a thermophilic glucose/xylose binding protein
Authors : Cuneo, M.J.; Hellinga, H.W.
Deposited on : 2008-02-05
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

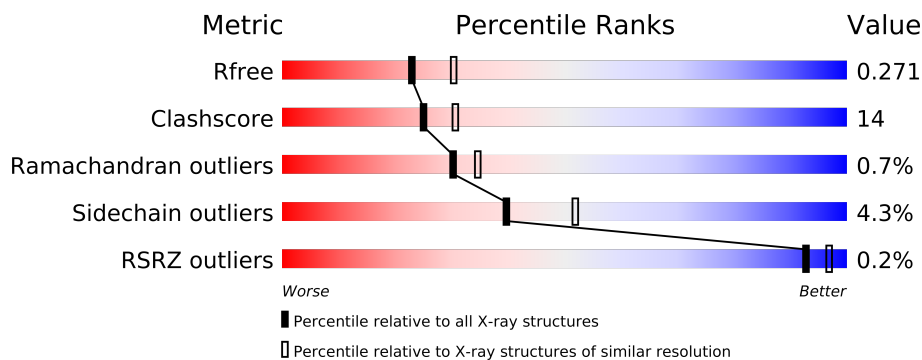
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	311	
1	B	311	
1	C	311	
1	D	311	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9588 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sugar ABC transporter, periplasmic sugar-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	305	Total	C	N	O	S	0	1	0
			2305	1478	369	443	15			
1	A	305	Total	C	N	O	S	0	1	0
			2305	1478	369	443	15			
1	C	305	Total	C	N	O	S	0	1	0
			2311	1482	372	442	15			
1	D	305	Total	C	N	O	S	0	0	0
			2302	1477	370	440	15			

There are 36 discrepancies between the modelled and reference sequences:

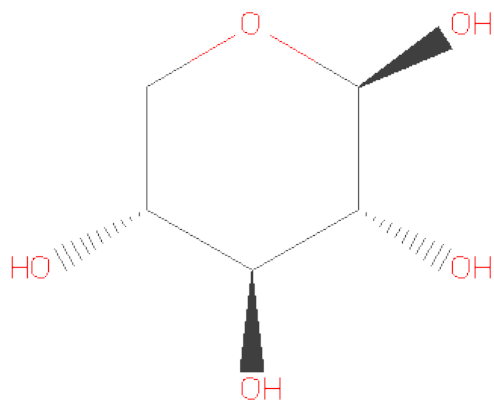
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP Q9WXW9
B	41	CYS	GLU	ENGINEERED	UNP Q9WXW9
B	163	CYS	GLU	ENGINEERED	UNP Q9WXW9
B	306	HIS	-	EXPRESSION TAG	UNP Q9WXW9
B	307	HIS	-	EXPRESSION TAG	UNP Q9WXW9
B	308	HIS	-	EXPRESSION TAG	UNP Q9WXW9
B	309	HIS	-	EXPRESSION TAG	UNP Q9WXW9
B	310	HIS	-	EXPRESSION TAG	UNP Q9WXW9
B	311	HIS	-	EXPRESSION TAG	UNP Q9WXW9
A	1	MET	-	INITIATING METHIONINE	UNP Q9WXW9
A	41	CYS	GLU	ENGINEERED	UNP Q9WXW9
A	163	CYS	GLU	ENGINEERED	UNP Q9WXW9
A	306	HIS	-	EXPRESSION TAG	UNP Q9WXW9
A	307	HIS	-	EXPRESSION TAG	UNP Q9WXW9
A	308	HIS	-	EXPRESSION TAG	UNP Q9WXW9
A	309	HIS	-	EXPRESSION TAG	UNP Q9WXW9
A	310	HIS	-	EXPRESSION TAG	UNP Q9WXW9
A	311	HIS	-	EXPRESSION TAG	UNP Q9WXW9
C	1	MET	-	INITIATING METHIONINE	UNP Q9WXW9
C	41	CYS	GLU	ENGINEERED	UNP Q9WXW9
C	163	CYS	GLU	ENGINEERED	UNP Q9WXW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	306	HIS	-	EXPRESSION TAG	UNP Q9WXW9
C	307	HIS	-	EXPRESSION TAG	UNP Q9WXW9
C	308	HIS	-	EXPRESSION TAG	UNP Q9WXW9
C	309	HIS	-	EXPRESSION TAG	UNP Q9WXW9
C	310	HIS	-	EXPRESSION TAG	UNP Q9WXW9
C	311	HIS	-	EXPRESSION TAG	UNP Q9WXW9
D	1	MET	-	INITIATING METHIONINE	UNP Q9WXW9
D	41	CYS	GLU	ENGINEERED	UNP Q9WXW9
D	163	CYS	GLU	ENGINEERED	UNP Q9WXW9
D	306	HIS	-	EXPRESSION TAG	UNP Q9WXW9
D	307	HIS	-	EXPRESSION TAG	UNP Q9WXW9
D	308	HIS	-	EXPRESSION TAG	UNP Q9WXW9
D	309	HIS	-	EXPRESSION TAG	UNP Q9WXW9
D	310	HIS	-	EXPRESSION TAG	UNP Q9WXW9
D	311	HIS	-	EXPRESSION TAG	UNP Q9WXW9

- Molecule 2 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is water.

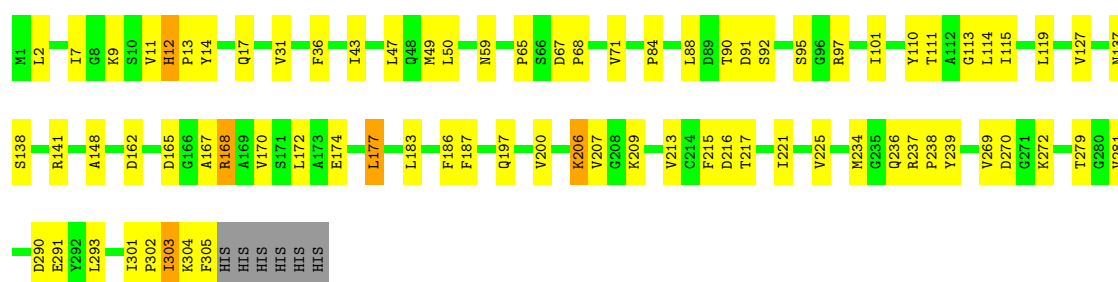
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	128	Total 128	O 128	0	0
3	C	61	Total 61	O 61	0	0
3	D	68	Total 68	O 68	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

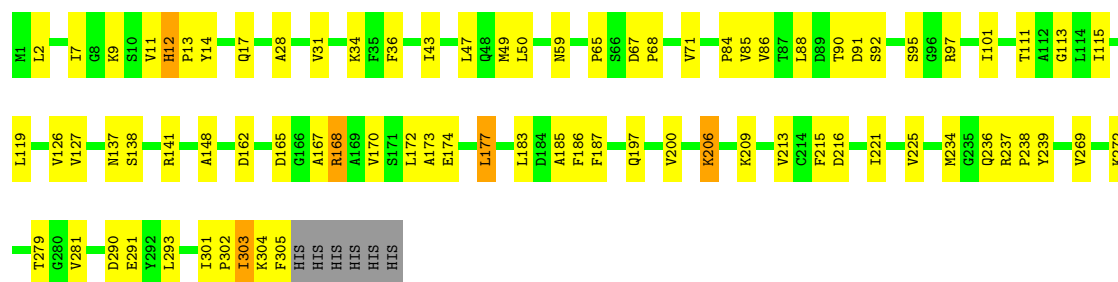
- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain B:



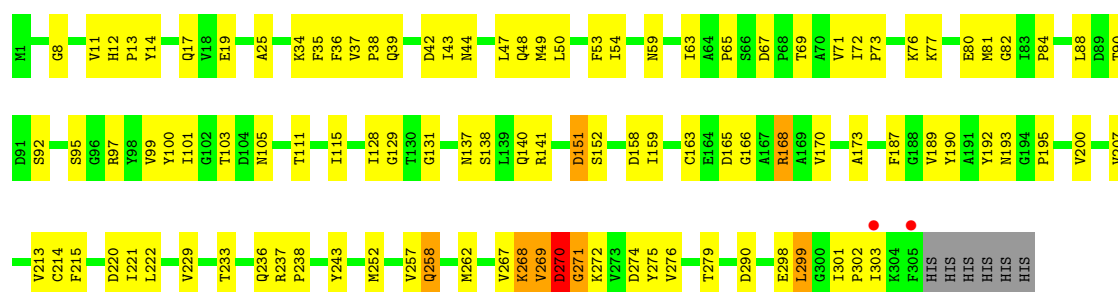
- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain A:



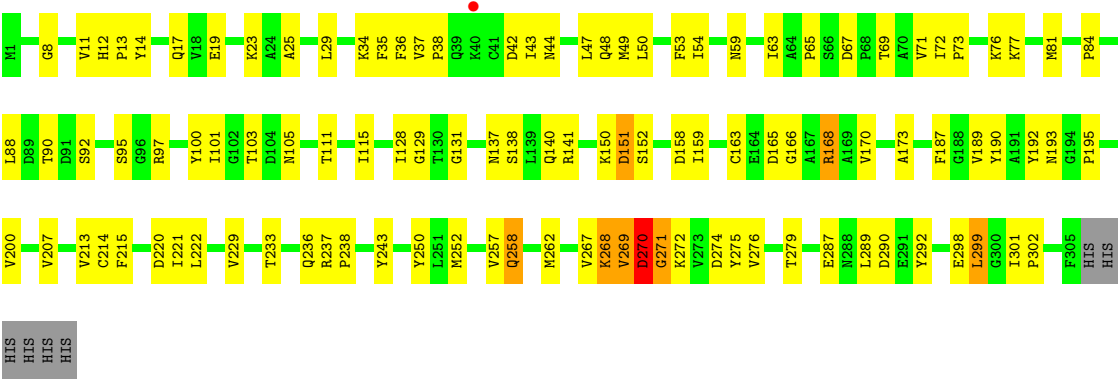
- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain C:



- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.10Å 75.75Å 100.52Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	19.87 – 2.30 19.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.87-2.30) 98.0 (19.87-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.30Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.281 0.205 , 0.271	Depositor DCC
R_{free} test set	2658 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 20.0	EDS
Estimated twinning fraction	0.460 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 53176 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9588	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP

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	0.37	0/2343	0.57	0/3178
1	B	0.38	0/2343	0.57	0/3178
1	C	0.36	0/2349	0.54	0/3184
1	D	0.36	0/2340	0.54	0/3172
All	All	0.37	0/9375	0.55	0/12712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2305	0	2350	62	0
1	B	2305	0	2350	60	0
1	C	2311	0	2370	67	0
1	D	2302	0	2363	69	0
2	C	10	0	10	0	0
2	D	10	0	10	0	0
3	A	88	0	0	4	0
3	B	128	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	61	0	0	1	0
3	D	68	0	0	4	0
All	All	9588	0	9453	258	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (258) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:MET:HB3	1:A:281:VAL:HG11	1.48	0.96
1:B:234:MET:HB3	1:B:281:VAL:HG11	1.49	0.93
1:C:269:VAL:O	1:C:270:ASP:HB2	1.77	0.81
1:D:269:VAL:O	1:D:270:ASP:HB2	1.77	0.81
1:D:8:GLY:HA3	1:D:37:VAL:HG12	1.70	0.72
1:B:168:ARG:HB3	1:B:168:ARG:HH11	1.55	0.72
1:A:168:ARG:HB3	1:A:168:ARG:HH11	1.55	0.72
1:D:36:PHE:CD2	1:D:49:MET:HG2	2.25	0.71
1:C:36:PHE:CD2	1:C:49:MET:HG2	2.25	0.71
1:C:8:GLY:HA3	1:C:37:VAL:HG12	1.72	0.70
1:D:252:MET:HG2	1:D:257:VAL:HA	1.74	0.70
1:B:186:PHE:HB3	1:B:197:GLN:NE2	2.07	0.70
1:B:206:LYS:HD2	1:B:209:LYS:HD2	1.75	0.69
1:A:206:LYS:HD2	1:A:209:LYS:HD2	1.76	0.68
1:D:287:GLU:HG2	3:D:532:HOH:O	1.93	0.68
1:C:252:MET:HG2	1:C:257:VAL:HA	1.76	0.68
1:A:186:PHE:HB3	1:A:197:GLN:NE2	2.09	0.68
1:B:14:TYR:CE1	1:B:238:PRO:HG3	2.29	0.67
1:A:14:TYR:CE1	1:A:238:PRO:HG3	2.30	0.67
1:C:166:GLY:O	1:C:170:VAL:HG23	1.95	0.65
1:B:36:PHE:CD2	1:B:49:MET:HG2	2.32	0.65
1:D:166:GLY:O	1:D:170:VAL:HG23	1.96	0.64
1:A:34:LYS:HE3	3:A:396:HOH:O	1.98	0.64
1:C:111:THR:O	1:C:115:ILE:HG12	1.98	0.64
1:A:36:PHE:CD2	1:A:49:MET:HG2	2.33	0.64
1:C:214:CYS:O	1:C:233:THR:HA	1.98	0.63
1:D:192:TYR:O	1:D:195:PRO:HD2	1.99	0.63
1:D:214:CYS:O	1:D:233:THR:HA	1.98	0.62
1:D:12:HIS:CG	1:D:13:PRO:HD2	2.34	0.62
1:A:2:LEU:HB2	1:A:31:VAL:HG23	1.81	0.62
1:C:128:ILE:HD12	1:C:159:ILE:HG12	1.81	0.62
1:A:115:ILE:O	1:A:119:LEU:HD12	1.98	0.62
1:C:192:TYR:O	1:C:195:PRO:HD2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:LYS:HG3	1:A:209:LYS:HB2	1.81	0.61
1:C:76:LYS:O	1:C:76:LYS:HD3	2.00	0.61
1:D:76:LYS:HD3	1:D:76:LYS:O	2.00	0.61
1:B:168:ARG:HH11	1:B:168:ARG:CG	2.13	0.61
1:B:2:LEU:HB2	1:B:31:VAL:HG23	1.83	0.60
1:D:111:THR:O	1:D:115:ILE:HG12	2.01	0.60
1:B:206:LYS:HG3	1:B:209:LYS:HB2	1.82	0.60
1:B:168:ARG:HH11	1:B:168:ARG:CB	2.15	0.60
1:C:67:ASP:O	1:C:71:VAL:HG13	2.02	0.59
1:A:162:ASP:HB3	1:A:172:LEU:HD12	1.84	0.59
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.15	0.59
1:D:67:ASP:O	1:D:71:VAL:HG13	2.02	0.59
1:A:168:ARG:CB	1:A:168:ARG:HH11	2.16	0.59
1:C:12:HIS:CG	1:C:13:PRO:HD2	2.37	0.59
1:B:115:ILE:O	1:B:119:LEU:HD12	2.01	0.59
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.85	0.59
1:B:162:ASP:HB3	1:B:172:LEU:HD12	1.85	0.59
1:D:141:ARG:HD3	1:D:215:PHE:CZ	2.38	0.58
1:D:72:ILE:HB	1:D:73:PRO:HD3	1.85	0.58
1:B:304:LYS:HD3	3:B:364:HOH:O	2.04	0.58
1:C:141:ARG:HD3	1:C:215:PHE:CZ	2.39	0.58
1:A:92:SER:OG	1:A:95:SER:HB3	2.04	0.58
1:C:43:ILE:O	1:C:47:LEU:HD13	2.03	0.58
1:D:43:ILE:O	1:D:47:LEU:HD13	2.04	0.58
1:B:137:ASN:O	1:B:141:ARG:HG3	2.04	0.57
1:B:92:SER:OG	1:B:95:SER:HB3	2.05	0.57
1:C:92:SER:OG	1:C:95:SER:HB3	2.05	0.56
1:C:258:GLN:HE21	1:C:258:GLN:HA	1.71	0.56
1:D:8:GLY:HA3	1:D:37:VAL:CG1	2.35	0.56
1:D:92:SER:OG	1:D:95:SER:HB3	2.05	0.56
1:C:207:VAL:HG22	1:C:229:VAL:HG13	1.88	0.55
1:C:11:VAL:HG23	1:C:38:PRO:O	2.07	0.55
1:A:12:HIS:CG	1:A:13:PRO:HD2	2.42	0.55
1:A:137:ASN:O	1:A:141:ARG:HG3	2.07	0.55
1:D:141:ARG:HD3	1:D:215:PHE:CE1	2.41	0.55
1:B:177:LEU:HD22	1:B:200:VAL:HG12	1.89	0.54
1:A:177:LEU:HD22	1:A:200:VAL:HG12	1.89	0.54
1:D:128:ILE:HD12	1:D:159:ILE:HG12	1.89	0.54
1:D:258:GLN:HA	1:D:258:GLN:HE21	1.73	0.54
1:B:221:ILE:O	1:B:225:VAL:HG23	2.08	0.54
1:A:221:ILE:O	1:A:225:VAL:HG23	2.08	0.54
1:D:23:LYS:HG2	3:D:514:HOH:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:8:GLY:HA3	1:C:37:VAL:CG1	2.38	0.53
1:B:59:ASN:O	1:B:84:PRO:HD2	2.08	0.53
1:A:68:PRO:HG2	3:A:322:HOH:O	2.09	0.53
1:D:173:ALA:HB3	1:D:200:VAL:HG21	1.90	0.53
1:B:12:HIS:CG	1:B:13:PRO:HD2	2.44	0.53
1:C:141:ARG:HD3	1:C:215:PHE:CE1	2.43	0.53
1:C:103:THR:OG1	1:C:236:GLN:HG2	2.08	0.53
1:B:186:PHE:HB3	1:B:197:GLN:CD	2.30	0.52
1:D:207:VAL:HG22	1:D:229:VAL:HG13	1.91	0.52
1:D:150:LYS:HD2	3:D:562:HOH:O	2.09	0.52
1:C:42:ASP:OD2	1:C:44:ASN:HB2	2.10	0.52
1:A:59:ASN:O	1:A:84:PRO:HD2	2.10	0.52
1:C:173:ALA:HB3	1:C:200:VAL:HG21	1.91	0.52
1:D:11:VAL:HG23	1:D:38:PRO:O	2.10	0.52
1:D:42:ASP:OD2	1:D:44:ASN:HB2	2.10	0.52
1:D:8:GLY:CA	1:D:37:VAL:HG12	2.39	0.52
1:C:151:ASP:OD2	1:C:152:SER:N	2.43	0.51
1:D:19:GLU:HB2	1:D:35:PHE:CE1	2.46	0.51
1:B:88:LEU:HA	1:B:101:ILE:O	2.10	0.51
1:D:12:HIS:HD2	1:D:192:TYR:CE1	2.29	0.51
1:D:14:TYR:CE1	1:D:238:PRO:HG3	2.46	0.51
1:C:12:HIS:HD2	1:C:192:TYR:CE1	2.30	0.50
1:D:207:VAL:HB	3:D:520:HOH:O	2.11	0.50
1:A:186:PHE:HB3	1:A:197:GLN:CD	2.31	0.50
1:A:141:ARG:HD3	1:A:215:PHE:CE1	2.46	0.50
1:A:43:ILE:HD13	1:A:67:ASP:H	1.75	0.50
1:A:17:GLN:O	1:A:239:TYR:HA	2.12	0.50
1:D:59:ASN:O	1:D:84:PRO:HD2	2.12	0.50
1:B:137:ASN:OD1	1:B:138:SER:N	2.45	0.50
1:B:141:ARG:HD3	1:B:215:PHE:CE1	2.46	0.50
1:B:237:ARG:HD2	1:B:279:THR:O	2.11	0.49
1:B:165:ASP:HB3	1:B:168:ARG:HD3	1.93	0.49
1:B:47:LEU:HD11	1:B:71:VAL:HA	1.94	0.49
1:B:43:ILE:HD13	1:B:67:ASP:H	1.76	0.49
1:D:151:ASP:OD2	1:D:152:SER:N	2.45	0.49
1:C:14:TYR:CE1	1:C:238:PRO:HG3	2.48	0.49
1:A:165:ASP:HB3	1:A:168:ARG:HD3	1.93	0.49
1:C:8:GLY:CA	1:C:37:VAL:HG12	2.42	0.49
1:A:115:ILE:O	1:A:119:LEU:CD1	2.60	0.49
1:B:17:GLN:O	1:B:239:TYR:HA	2.13	0.49
1:C:59:ASN:O	1:C:84:PRO:HD2	2.13	0.49
1:A:88:LEU:HA	1:A:101:ILE:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:105:ASN:HB2	1:C:140:GLN:OE1	2.12	0.48
1:B:9:LYS:HZ2	1:B:90:THR:HG21	1.78	0.48
1:A:47:LEU:HD11	1:A:71:VAL:HA	1.96	0.48
1:B:2:LEU:CB	1:B:31:VAL:HG23	2.44	0.48
1:D:267:VAL:HG23	1:D:267:VAL:O	2.14	0.48
1:D:275:TYR:O	1:D:276:VAL:HG23	2.13	0.48
1:C:19:GLU:HB2	1:C:35:PHE:CE1	2.49	0.47
1:D:50:LEU:O	1:D:54:ILE:HG13	2.13	0.47
1:A:65:PRO:HB3	1:A:71:VAL:HG11	1.95	0.47
1:A:137:ASN:OD1	1:A:138:SER:N	2.47	0.47
1:B:67:ASP:HA	1:B:68:PRO:HD2	1.69	0.47
1:C:50:LEU:O	1:C:54:ILE:HG13	2.14	0.47
1:C:267:VAL:HG23	1:C:267:VAL:O	2.15	0.47
1:D:12:HIS:ND1	1:D:13:PRO:HD2	2.30	0.47
1:B:187:PHE:HA	1:B:213:VAL:O	2.15	0.47
1:A:303:ILE:HG23	1:A:303:ILE:O	2.14	0.47
1:B:270:ASP:HB2	3:B:420:HOH:O	2.14	0.47
1:C:100:TYR:HB3	1:C:276:VAL:HG22	1.97	0.47
1:B:303:ILE:O	1:B:303:ILE:HG23	2.14	0.46
1:B:115:ILE:O	1:B:119:LEU:CD1	2.63	0.46
1:B:215:PHE:O	1:B:216:ASP:HB2	2.14	0.46
1:C:275:TYR:O	1:C:276:VAL:HG23	2.14	0.46
1:D:138:SER:HB2	1:D:190:TYR:CE1	2.50	0.46
1:B:113:GLY:HA3	1:B:148:ALA:HB3	1.98	0.46
1:A:113:GLY:HA3	1:A:148:ALA:HB3	1.98	0.46
1:B:168:ARG:NH1	1:B:168:ARG:CG	2.78	0.46
1:C:195:PRO:HG3	1:C:221:ILE:CG1	2.44	0.46
1:D:100:TYR:HB3	1:D:276:VAL:HG22	1.98	0.46
1:D:267:VAL:CG2	1:D:274:ASP:HB3	2.46	0.46
1:A:111:THR:HG22	1:A:234:MET:HE1	1.97	0.46
1:A:2:LEU:CB	1:A:31:VAL:HG23	2.43	0.46
1:D:103:THR:OG1	1:D:236:GLN:HG2	2.15	0.46
1:D:34:LYS:HB3	1:D:53:PHE:CZ	2.50	0.46
1:C:267:VAL:CG2	1:C:274:ASP:HB3	2.46	0.46
1:C:17:GLN:OE1	1:C:238:PRO:HG2	2.16	0.46
1:A:170:VAL:O	1:A:174:GLU:HG3	2.16	0.46
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.79	0.46
1:C:137:ASN:O	1:C:141:ARG:HG3	2.16	0.46
1:C:138:SER:HB2	1:C:190:TYR:CE1	2.50	0.46
1:A:67:ASP:HA	1:A:68:PRO:HD2	1.71	0.45
1:A:88:LEU:HD23	1:A:88:LEU:H	1.81	0.45
1:D:105:ASN:HB2	1:D:140:GLN:OE1	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:237:ARG:HD2	1:A:279:THR:O	2.15	0.45
1:D:220:ASP:N	1:D:220:ASP:OD2	2.45	0.45
1:D:77:LYS:O	1:D:81:MET:HG2	2.17	0.45
1:B:111:THR:HG22	1:B:234:MET:HE1	1.98	0.45
1:A:168:ARG:CG	1:A:168:ARG:NH1	2.79	0.45
1:C:258:GLN:HG3	1:C:262:MET:CE	2.47	0.45
1:A:9:LYS:NZ	1:A:90:THR:HG21	2.32	0.45
1:C:34:LYS:HB3	1:C:53:PHE:CZ	2.52	0.45
1:B:91:ASP:OD1	1:B:92:SER:N	2.50	0.44
1:B:65:PRO:HD2	1:B:90:THR:O	2.16	0.44
1:D:237:ARG:HG3	1:D:279:THR:O	2.17	0.44
1:C:301:ILE:HA	1:C:302:PRO:HD3	1.86	0.44
1:A:7:ILE:HD12	1:A:50:LEU:HD13	2.00	0.44
1:B:168:ARG:NH1	1:B:168:ARG:HG2	2.33	0.44
1:C:220:ASP:OD2	1:C:220:ASP:N	2.47	0.44
1:A:215:PHE:O	1:A:216:ASP:HB2	2.16	0.44
1:C:303:ILE:HA	1:C:303:ILE:HD13	1.87	0.44
1:C:268:LYS:HE3	1:C:271:GLY:HA2	1.99	0.44
1:B:7:ILE:HD12	1:B:50:LEU:HD13	2.00	0.44
1:B:9:LYS:NZ	1:B:90:THR:HG21	2.33	0.43
1:C:14:TYR:O	1:C:17:GLN:HB2	2.18	0.43
1:B:127:VAL:HG23	1:B:183:LEU:HD13	2.00	0.43
1:B:290[B]:ASP:OD1	1:B:291:GLU:N	2.51	0.43
1:C:195:PRO:HG3	1:C:221:ILE:HG12	2.00	0.43
1:D:138:SER:HB2	1:D:190:TYR:HE1	1.83	0.43
1:A:290[B]:ASP:OD1	1:A:291:GLU:N	2.51	0.43
1:D:268:LYS:HE3	1:D:271:GLY:HA2	1.99	0.43
1:D:195:PRO:HG3	1:D:221:ILE:CG1	2.47	0.43
1:B:88:LEU:H	1:B:88:LEU:HD23	1.83	0.43
1:C:237:ARG:HG3	1:C:279:THR:O	2.18	0.43
1:B:170:VAL:O	1:B:174:GLU:HG3	2.18	0.43
1:D:25:ALA:HB2	1:D:243:TYR:HA	2.00	0.43
1:C:12:HIS:ND1	1:C:13:PRO:HD2	2.34	0.43
1:C:25:ALA:HB2	1:C:243:TYR:HA	2.00	0.43
1:A:168:ARG:HH11	1:A:168:ARG:HG2	1.81	0.43
1:D:137:ASN:O	1:D:141:ARG:HG3	2.19	0.43
1:A:91:ASP:OD1	1:A:92:SER:N	2.52	0.42
1:A:173:ALA:HB3	1:A:200:VAL:HG21	2.01	0.42
1:B:269:VAL:O	1:B:272:LYS:HB3	2.19	0.42
1:D:168:ARG:HE	1:D:168:ARG:HB2	1.71	0.42
1:A:126:VAL:HG22	1:A:185:ALA:HB3	2.01	0.42
1:A:85:VAL:HG12	1:A:86:VAL:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:65:PRO:HB3	1:B:71:VAL:HG11	2.00	0.42
1:C:131:GLY:O	1:C:163:CYS:HA	2.19	0.42
1:A:168:ARG:HG2	1:A:168:ARG:NH1	2.35	0.42
1:C:63:ILE:O	1:C:65:PRO:HD3	2.19	0.42
1:C:138:SER:HB2	1:C:190:TYR:HE1	1.85	0.42
1:C:168:ARG:HE	1:C:168:ARG:HB2	1.71	0.42
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.85	0.42
1:D:17:GLN:OE1	1:D:238:PRO:HG2	2.19	0.42
1:C:189:VAL:HG12	1:C:190:TYR:HD1	1.83	0.42
1:C:77:LYS:O	1:C:81:MET:HG2	2.20	0.42
1:D:76:LYS:C	1:D:76:LYS:HD3	2.40	0.42
1:D:14:TYR:O	1:D:17:GLN:HB2	2.20	0.42
1:C:76:LYS:HD3	1:C:76:LYS:C	2.40	0.42
1:A:65:PRO:HD2	1:A:90:THR:O	2.19	0.42
1:D:131:GLY:O	1:D:163:CYS:HA	2.19	0.42
1:C:39:GLN:HB3	3:C:546:HOH:O	2.18	0.42
1:B:207:VAL:HG23	3:B:402:HOH:O	2.19	0.42
1:A:187:PHE:HA	1:A:213:VAL:O	2.20	0.42
1:C:88:LEU:HA	1:C:101:ILE:O	2.19	0.42
1:D:301:ILE:HA	1:D:302:PRO:HD3	1.87	0.42
1:D:165:ASP:HB3	1:D:168:ARG:HB3	2.02	0.42
1:D:129:GLY:C	1:D:193:ASN:ND2	2.73	0.42
1:B:236:GLN:C	1:B:238:PRO:HD3	2.40	0.42
1:D:289:LEU:O	1:D:292:TYR:HB3	2.20	0.42
1:D:299:LEU:HD23	1:D:299:LEU:HA	1.87	0.41
1:D:258:GLN:HG3	1:D:262:MET:CE	2.50	0.41
1:B:11:VAL:O	1:B:12:HIS:O	2.38	0.41
1:A:301:ILE:HA	1:A:302:PRO:HD3	1.92	0.41
1:A:269:VAL:O	1:A:272:LYS:HB3	2.21	0.41
1:A:206:LYS:HB2	1:A:206:LYS:HZ2	1.86	0.41
1:A:177:LEU:HD22	1:A:200:VAL:CG1	2.50	0.41
1:C:99:VAL:HG12	1:C:100:TYR:N	2.35	0.41
1:B:293:LEU:HD22	1:B:303:ILE:HG21	2.01	0.41
1:D:189:VAL:HG12	1:D:190:TYR:HD1	1.84	0.41
1:A:127:VAL:HG23	1:A:183:LEU:HD13	2.02	0.41
1:A:11:VAL:O	1:A:12:HIS:O	2.38	0.41
1:B:301:ILE:HA	1:B:302:PRO:HD3	1.92	0.41
1:A:28:ALA:HB2	3:A:330:HOH:O	2.19	0.41
1:D:195:PRO:HG3	1:D:221:ILE:HG12	2.02	0.41
1:D:29:LEU:HD13	1:D:250:TYR:CG	2.55	0.41
1:D:187:PHE:HA	1:D:213:VAL:O	2.19	0.41
1:C:187:PHE:HA	1:C:213:VAL:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:GLN:C	1:A:238:PRO:HD3	2.40	0.41
1:B:303:ILE:HA	1:B:303:ILE:HD12	1.80	0.41
1:C:80:GLU:C	1:C:82:GLY:H	2.24	0.41
1:C:65:PRO:HB3	1:C:71:VAL:HG11	2.02	0.41
1:A:293:LEU:HD22	1:A:303:ILE:HG21	2.02	0.41
1:C:165:ASP:HB3	1:C:168:ARG:HB3	2.03	0.41
1:A:304:LYS:HD3	3:A:379:HOH:O	2.20	0.41
1:D:88:LEU:HA	1:D:101:ILE:O	2.21	0.41
1:B:165:ASP:OD2	1:B:167:ALA:HB3	2.21	0.40
1:D:63:ILE:O	1:D:65:PRO:HD3	2.20	0.40
1:A:165:ASP:OD2	1:A:167:ALA:HB3	2.22	0.40
1:B:110:TYR:CE1	1:B:114:LEU:HD21	2.56	0.40
1:B:177:LEU:HD22	1:B:200:VAL:CG1	2.52	0.40
1:C:129:GLY:C	1:C:193:ASN:ND2	2.75	0.40
1:D:65:PRO:HB3	1:D:71:VAL:HG11	2.03	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	304/311 (98%)	290 (95%)	13 (4%)	1 (0%)	50 60
1	B	304/311 (98%)	291 (96%)	12 (4%)	1 (0%)	50 60
1	C	304/311 (98%)	275 (90%)	26 (9%)	3 (1%)	22 23
1	D	303/311 (97%)	278 (92%)	22 (7%)	3 (1%)	22 23
All	All	1215/1244 (98%)	1134 (93%)	73 (6%)	8 (1%)	30 34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	HIS
1	A	12	HIS
1	C	270	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	270	ASP
1	C	271	GLY
1	D	271	GLY
1	C	269	VAL
1	D	269	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	249/256 (97%)	243 (98%)	6 (2%)	61	79
1	B	249/256 (97%)	242 (97%)	7 (3%)	56	73
1	C	251/256 (98%)	235 (94%)	16 (6%)	25	31
1	D	250/256 (98%)	235 (94%)	15 (6%)	27	35
All	All	999/1024 (98%)	955 (96%)	44 (4%)	40	51

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	ARG
1	B	168	ARG
1	B	177	LEU
1	B	206	LYS
1	B	217	THR
1	B	303	ILE
1	B	305	PHE
1	A	97	ARG
1	A	168	ARG
1	A	177	LEU
1	A	206	LYS
1	A	303	ILE
1	A	305	PHE
1	C	48[A]	GLN
1	C	48[B]	GLN
1	C	69	THR
1	C	90	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	97	ARG
1	C	151	ASP
1	C	158	ASP
1	C	168	ARG
1	C	222	LEU
1	C	258	GLN
1	C	268	LYS
1	C	270	ASP
1	C	272	LYS
1	C	290	ASP
1	C	298	GLU
1	C	299	LEU
1	D	48	GLN
1	D	69	THR
1	D	90	THR
1	D	97	ARG
1	D	151	ASP
1	D	158	ASP
1	D	168	ARG
1	D	222	LEU
1	D	258	GLN
1	D	268	LYS
1	D	270	ASP
1	D	272	LYS
1	D	290	ASP
1	D	298	GLU
1	D	299	LEU

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

Mol	Chain	Res	Type
1	B	20	GLN
1	B	48	GLN
1	A	20	GLN
1	A	44	ASN
1	A	48	GLN
1	C	193	ASN
1	C	258	GLN
1	D	48	GLN
1	D	193	ASN
1	D	258	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	XYP	C	500	-	10,10,10	1.67	1 (10%)	14,14,14	0.98	1 (7%)
2	XYP	D	501	-	10,10,10	1.65	1 (10%)	14,14,14	0.83	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	XYP	C	500	-	-	0/0/17/17	0/1/1/1
2	XYP	D	501	-	-	0/0/17/17	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	XYP	O5B-C1B	-4.68	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	XYP	O5B-C1B	-4.50	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	XYP	C5B-C4B-C3B	3.23	113.78	109.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	305/311 (98%)	-0.42	0	100 100	12, 34, 58, 82	0
1	B	305/311 (98%)	-0.40	0	100 100	14, 34, 59, 82	0
1	C	305/311 (98%)	-0.27	2 (0%)	84 91	19, 40, 72, 108	0
1	D	305/311 (98%)	-0.31	1 (0%)	91 96	20, 40, 73, 105	0
All	All	1220/1244 (98%)	-0.35	3 (0%)	93 97	12, 37, 66, 108	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	PHE	2.7
1	C	303	ILE	2.4
1	D	40	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	XYP	D	501	10/10	0.11	0.57	17,34,41,52	0
2	XYP	C	500	10/10	0.08	-1.07	15,35,47,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.