



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:28 PM UTC

PDB ID : 3C6Q / pdb_00003c6q
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 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

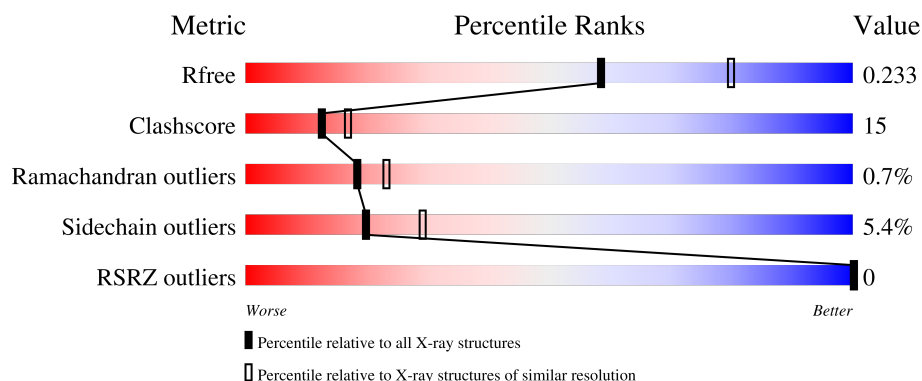
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	311	69% 26% ..
1	B	311	70% 26% ..
1	C	311	60% 34% ..
1	D	311	60% 34% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9588 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 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:

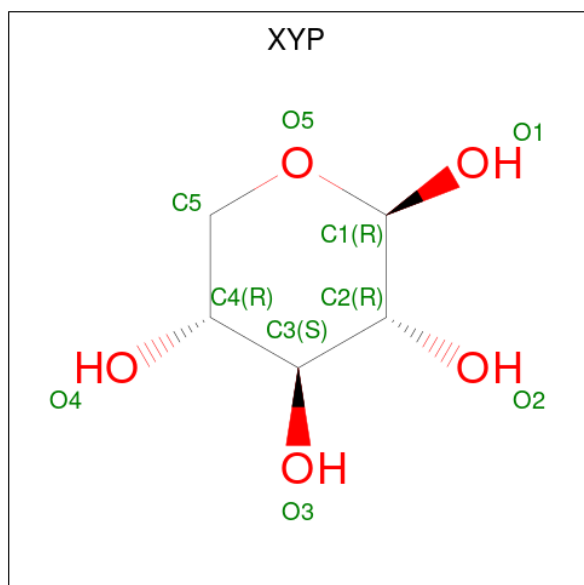
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9WXW9
B	41	CYS	GLU	engineered mutation	UNP Q9WXW9
B	163	CYS	GLU	engineered mutation	UNP Q9WXW9
B	306	HIS	-	expression tag	UNP Q9WXW9
B	307	HIS	-	expression tag	UNP Q9WXW9
B	308	HIS	-	expression tag	UNP Q9WXW9
B	309	HIS	-	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 mutation	UNP Q9WXW9
A	163	CYS	GLU	engineered mutation	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 mutation	UNP Q9WXW9
C	163	CYS	GLU	engineered mutation	UNP Q9WXW9

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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 mutation	UNP Q9WXW9
D	163	CYS	GLU	engineered mutation	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 beta-D-xylopyranose (CCD ID: XYP) (formula: C₅H₁₀O₅).



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		

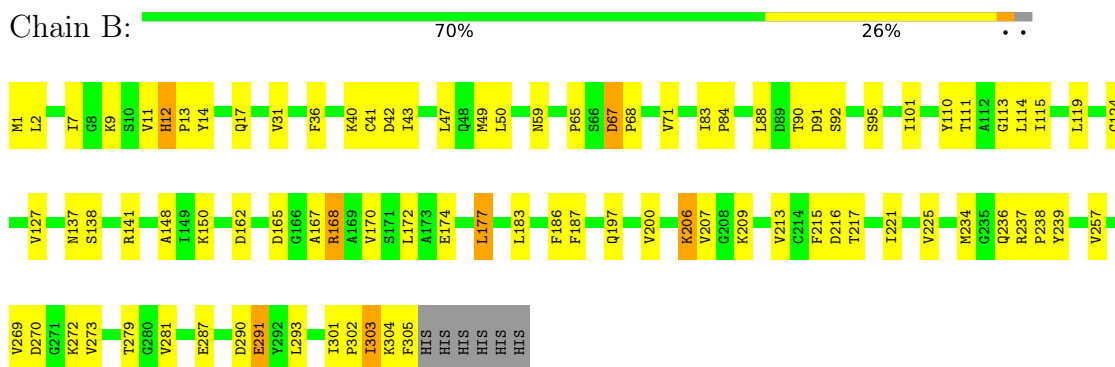
- Molecule 3 is water.

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

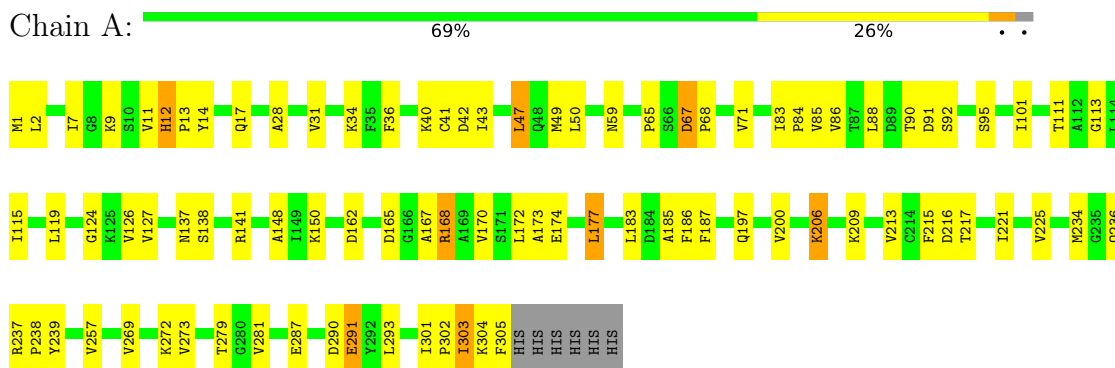
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

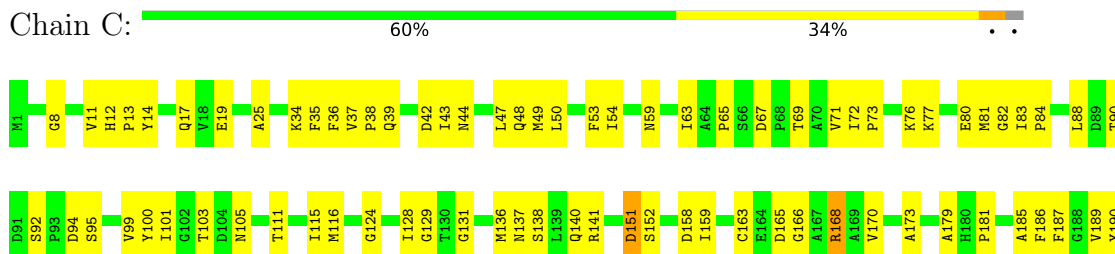
- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein

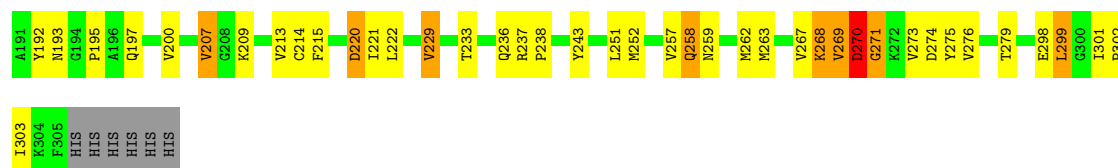


- Molecule 1: Sugar ABC transporter, periplasmic sugar-binding protein



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





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

Chain D: 60% 34%



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) 98.1 (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 (Not available) , 0.233	Depositor DCC
R_{free} test set	2659 reflections (5.00%)	wwPDB-VP
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 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.460 for h,-k,-l	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.

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: 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	0.49	0/2343	0.90	5/3178 (0.2%)
1	B	0.50	0/2343	0.90	5/3178 (0.2%)
1	C	0.45	0/2349	0.89	5/3184 (0.2%)
1	D	0.45	0/2340	0.89	6/3172 (0.2%)
All	All	0.48	0/9375	0.90	21/12712 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	GLY	N-CA-C	7.07	120.56	110.46
1	C	124	GLY	N-CA-C	6.60	119.89	110.46
1	D	83	ILE	CA-C-N	6.38	126.73	119.83
1	D	83	ILE	C-N-CA	6.38	126.73	119.83
1	C	83	ILE	CA-C-N	6.22	126.55	119.83
1	C	83	ILE	C-N-CA	6.22	126.55	119.83
1	B	83	ILE	CA-C-N	5.57	125.75	119.90
1	B	83	ILE	C-N-CA	5.57	125.75	119.90
1	A	83	ILE	CA-C-N	5.48	125.66	119.90
1	A	83	ILE	C-N-CA	5.48	125.66	119.90
1	B	67	ASP	CA-C-N	5.36	125.69	119.47
1	B	67	ASP	C-N-CA	5.36	125.69	119.47
1	B	124	GLY	N-CA-C	5.35	118.21	111.09
1	D	237	ARG	CA-C-N	5.26	124.89	119.05
1	D	237	ARG	C-N-CA	5.26	124.89	119.05
1	A	67	ASP	CA-C-N	5.25	125.57	119.47
1	A	67	ASP	C-N-CA	5.25	125.57	119.47
1	C	229	VAL	N-CA-C	-5.24	107.30	111.81
1	D	229	VAL	N-CA-C	-5.18	107.36	111.81
1	A	124	GLY	N-CA-C	5.16	117.95	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	185	ALA	N-CA-C	5.01	116.13	108.42

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	2305	0	2350	65	0
1	B	2305	0	2350	62	0
1	C	2311	0	2370	78	0
1	D	2302	0	2363	80	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	88	0	0	5	0
3	B	128	0	0	4	0
3	C	61	0	0	1	0
3	D	68	0	0	4	0
All	All	9588	0	9433	285	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 15.

All (285) 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: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:HH11	1:B:168:ARG:HB3	1.55	0.72
1:A:168:ARG:HH11	1:A:168:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:115:ILE:O	1:A:119:LEU:HD12	1.98	0.62
1:C:128:ILE:HD12	1:C:159:ILE:HG12	1.81	0.62
1:C:192:TYR:O	1:C:195:PRO:HD2	2.00	0.62
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:O	1:D:76:LYS:HD3	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:A:162:ASP:HB3	1:A:172:LEU:HD12	1.84	0.59
1:C:67:ASP:O	1:C:71:VAL:HG13	2.02	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:HH11	1:A:168:ARG:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:HB	1:D:73:PRO:HD3	1.85	0.58
1:D:141:ARG:HD3	1:D:215:PHE:CZ	2.38	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:D:251:LEU:HD13	1:D:263:MET:HE1	1.85	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:B:186:PHE:HB3	1:B:197:GLN:CD	2.30	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:A:111:THR:HG22	1:A:234:MET:HE1	1.88	0.56
1:A:186:PHE:HB3	1:A:197:GLN:CD	2.31	0.55
1:C:207:VAL:HG22	1:C:229:VAL:HG13	1.88	0.55
1:A:12:HIS:CG	1:A:13:PRO:HD2	2.42	0.55
1:C:11:VAL:HG23	1:C:38:PRO:O	2.07	0.55
1:C:251:LEU:HD13	1:C:263:MET:HE1	1.88	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:HE21	1:D:258:GLN:HA	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
1:C:8:GLY:HA3	1:C:37:VAL:CG1	2.38	0.53
1:C:258:GLN:HG3	1:C:262:MET:HE2	1.90	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:136:MET:HE2	1:D:140:GLN:NE2	2.23	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:B:111:THR:HG22	1:B:234:MET:HE1	1.91	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:D:136:MET:HE2	1:D:140:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	3:A:358:HOH:O	2.09	0.52
1:C:136:MET:HE2	1:C:140:GLN:HE21	1.75	0.52
1:D:207:VAL:HG22	1:D:229:VAL:HG13	1.91	0.52
1:C:42:ASP:OD2	1:C:44:ASN:HB2	2.10	0.52
1:D:150:LYS:HD2	3:D:562:HOH:O	2.09	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:17:GLN:O	1:A:239:TYR:HA	2.12	0.50
1:A:43:ILE:HD13	1:A:67:ASP:H	1.75	0.50
1:A:141:ARG:HD3	1:A:215:PHE:CE1	2.46	0.50
1:C:136:MET:HE2	1:C:140:GLN:NE2	2.25	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:D:258:GLN:HG3	1:D:262:MET:HE2	1.94	0.50
1:B:237:ARG:HD2	1:B:279:THR:O	2.11	0.49
1:B:43:ILE:HD13	1:B:67:ASP:H	1.76	0.49
1:B:47:LEU:HD11	1:B:71:VAL:HA	1.94	0.49
1:B:165:ASP:HB3	1:B:168:ARG:HD3	1.93	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:B:17:GLN:O	1:B:239:TYR:HA	2.13	0.49
1:A:115:ILE:O	1:A:119:LEU:CD1	2.60	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: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
1:C:105:ASN:HB2	1:C:140:GLN:OE1	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:TYR:O	1:D:276:VAL:HG23	2.13	0.48
1:D:81:MET:HE3	1:D:81:MET:HB3	1.72	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:B:1:MET:HE2	3:B:387:HOH:O	2.14	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:O	1:C:267:VAL:HG23	2.15	0.47
1:D:76:LYS:HD3	1:D:76:LYS:C	2.40	0.47
1:B:187:PHE:HA	1:B:213:VAL:O	2.15	0.47
1:B:236:GLN:C	1:B:238:PRO:HD3	2.40	0.47
1:A:303:ILE:HG23	1:A:303:ILE:O	2.14	0.47
1:C:76:LYS:HD3	1:C:76:LYS:C	2.40	0.47
1:D:12:HIS:ND1	1:D:13:PRO:HD2	2.30	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:HG23	1:B:303:ILE:O	2.14	0.46
1:D:129:GLY:C	1:D:193:ASN:ND2	2.73	0.46
1:B:113:GLY:HA3	1:B:148:ALA:HB3	1.98	0.46
1:B:115:ILE:O	1:B:119:LEU:CD1	2.63	0.46
1:A:113:GLY:HA3	1:A:148:ALA:HB3	1.98	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:168:ARG:CG	1:B:168:ARG:NH1	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:B:215:PHE:O	1:B:216:ASP:HB2	2.14	0.46
1:D:267:VAL:CG2	1:D:274:ASP:HB3	2.46	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:A:170:VAL:O	1:A:174:GLU:HG3	2.16	0.46
1:C:17:GLN:OE1	1:C:238:PRO:HG2	2.16	0.46
1:B:168:ARG:HH11	1:B:168:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLN:C	1:A:238:PRO:HD3	2.40	0.45
1:C:80:GLU:C	1:C:82:GLY:H	2.24	0.45
1:D:105:ASN:HB2	1:D:140:GLN:OE1	2.15	0.45
1:A:237:ARG:HD2	1:A:279:THR:O	2.15	0.45
1:C:81:MET:HE3	1:C:81:MET:HB3	1.74	0.45
1:D:220:ASP:OD2	1:D:220:ASP:N	2.45	0.45
1:C:129:GLY:C	1:C:193:ASN:ND2	2.75	0.45
1:D:77:LYS:O	1:D:81:MET:HG2	2.17	0.45
1:A:168:ARG:CG	1:A:168:ARG:NH1	2.79	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:C:258:GLN:HG3	1:C:262:MET:CE	2.47	0.45
1:B:65:PRO:HD2	1:B:90:THR:O	2.16	0.44
1:B:91:ASP:OD1	1:B:92:SER:N	2.50	0.44
1:C:116:MET:HE2	1:C:213:VAL:HB	1.99	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:D:80:GLU:C	1:D:82:GLY:H	2.25	0.44
1:D:116:MET:HE2	1:D:213:VAL:HB	2.00	0.44
1:C:303:ILE:HD13	1:C:303:ILE:HA	1.87	0.44
1:B:7:ILE:HD12	1:B:50:LEU:HD13	2.00	0.44
1:C:268:LYS:HE3	1:C:271:GLY:HA2	1.99	0.44
1:B:9:LYS:NZ	1:B:90:THR:HG21	2.33	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:14:TYR:O	1:C:17:GLN:HB2	2.18	0.43
1:A:290[B]:ASP:OD1	1:A: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:D:268:LYS:HE3	1:D:271:GLY:HA2	1.99	0.43
1:D:186:PHE:HB3	1:D:197:GLN:CD	2.43	0.43
1:D:195:PRO:HG3	1:D:221:ILE:CG1	2.47	0.43
1:B:88:LEU:HD23	1:B:88:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ALA:HB2	1:C:243:TYR:HA	2.00	0.43
1:D:268:LYS:O	1:D:269:VAL:C	2.62	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:C:186:PHE:HB3	1:C:197:GLN:CD	2.44	0.43
1:B:269:VAL:O	1:B:272:LYS:HB3	2.19	0.42
1:A:42:ASP:C	1:A:42:ASP:OD1	2.61	0.42
1:A:85:VAL:HG12	1:A:86:VAL:N	2.34	0.42
1:A:91:ASP:OD1	1:A:92:SER:N	2.52	0.42
1:A:126:VAL:HG22	1:A:185:ALA:HB3	2.01	0.42
1:A:173:ALA:HB3	1:A:200:VAL:HG21	2.01	0.42
1:D:168:ARG:HE	1:D:168:ARG:HB2	1.71	0.42
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:C:268:LYS:O	1:C:269:VAL:C	2.62	0.42
1:B:40:LYS:O	1:B:41:CYS:C	2.63	0.42
1:A:168:ARG:NH1	1:A:168:ARG:HG2	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:77:LYS:O	1:C:81:MET:HG2	2.20	0.42
1:C:189:VAL:HG12	1:C:190:TYR:HD1	1.83	0.42
1:D:14:TYR:O	1:D:17:GLN:HB2	2.20	0.42
1:B:207:VAL:HG23	3:B:402:HOH:O	2.19	0.42
1:A:65:PRO:HD2	1:A:90:THR:O	2.19	0.42
1:C:39:GLN:HB3	3:C:546:HOH:O	2.18	0.42
1:D:131:GLY:O	1:D:163:CYS:HA	2.19	0.42
1:D:179:ALA:C	1:D:181:PRO:HD3	2.45	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:289:LEU:O	1:D:292:TYR:HB3	2.20	0.42
1:C:207:VAL:C	1:C:209:LYS:H	2.27	0.41
1:D:299:LEU:HD23	1:D:299:LEU:HA	1.87	0.41
1:B:42:ASP:OD1	1:B:42:ASP:C	2.62	0.41
1:C:179:ALA:C	1:C:181:PRO:HD3	2.45	0.41
1:B:11:VAL:O	1:B:12:HIS:O	2.38	0.41
1:A:269:VAL:O	1:A:272:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HA	1:A:302:PRO:HD3	1.92	0.41
1:D:207:VAL:C	1:D:209:LYS:H	2.28	0.41
1:D:258:GLN:HG3	1:D:262:MET:CE	2.50	0.41
1:B:293:LEU:HD22	1:B:303:ILE:HG21	2.01	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:A:127:VAL:HG23	1:A:183:LEU:HD13	2.02	0.41
1:D:189:VAL:HG12	1:D:190:TYR:HD1	1.84	0.41
1:B:301:ILE:HA	1:B:302:PRO:HD3	1.92	0.41
1:A:11:VAL:O	1:A:12:HIS:O	2.38	0.41
1:A:28:ALA:HB2	3:A:330:HOH:O	2.19	0.41
1:C:187:PHE:HA	1:C:213:VAL:O	2.19	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:D:195:PRO:HG3	1:D:221:ILE:HG12	2.02	0.41
1:B:303:ILE:HD12	1:B:303:ILE:HA	1.80	0.41
1:A:11:VAL:O	1:A:12:HIS:C	2.64	0.41
1:A:293:LEU:HD22	1:A:303:ILE:HG21	2.02	0.41
1:C:65:PRO:HB3	1:C:71:VAL:HG11	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:B:110:TYR:CE1	1:B:114:LEU:HD21	2.56	0.40
1:A:40:LYS:O	1:A:41:CYS:C	2.65	0.40
1:A:165:ASP:OD2	1:A:167:ALA:HB3	2.22	0.40
1:B:177:LEU:HD22	1:B:200:VAL:CG1	2.52	0.40
1:C:258:GLN:O	1:C:259:ASN:C	2.64	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 [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	304/311 (98%)	290 (95%)	13 (4%)	1 (0%)	36	46
1	B	304/311 (98%)	291 (96%)	12 (4%)	1 (0%)	36	46
1	C	304/311 (98%)	275 (90%)	26 (9%)	3 (1%)	12	15
1	D	303/311 (97%)	278 (92%)	22 (7%)	3 (1%)	12	15
All	All	1215/1244 (98%)	1134 (93%)	73 (6%)	8 (1%)	18	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	HIS
1	A	12	HIS
1	C	270	ASP
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%)	237 (95%)	12 (5%)	23	35
1	B	249/256 (97%)	238 (96%)	11 (4%)	25	38
1	C	251/256 (98%)	234 (93%)	17 (7%)	14	20
1	D	250/256 (98%)	235 (94%)	15 (6%)	17	25
All	All	999/1024 (98%)	944 (94%)	55 (6%)	20	28

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	LYS
1	B	168	ARG
1	B	177	LEU
1	B	206	LYS
1	B	217	THR
1	B	257	VAL
1	B	273	VAL
1	B	287	GLU
1	B	291	GLU
1	B	303	ILE
1	B	305	PHE
1	A	47	LEU
1	A	150	LYS
1	A	168	ARG
1	A	177	LEU
1	A	206	LYS
1	A	217	THR
1	A	257	VAL
1	A	273	VAL
1	A	287	GLU
1	A	291	GLU
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
1	C	94	ASP
1	C	151	ASP
1	C	158	ASP
1	C	168	ARG
1	C	207	VAL
1	C	220	ASP
1	C	222	LEU
1	C	258	GLN
1	C	268	LYS
1	C	270	ASP
1	C	273	VAL
1	C	298	GLU
1	C	299	LEU
1	D	48	GLN
1	D	69	THR
1	D	90	THR

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Mol	Chain	Res	Type
1	D	151	ASP
1	D	158	ASP
1	D	168	ARG
1	D	207	VAL
1	D	220	ASP
1	D	222	LEU
1	D	258	GLN
1	D	268	LYS
1	D	270	ASP
1	D	273	VAL
1	D	298	GLU
1	D	299	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	GLN
1	B	140	GLN
1	B	193	ASN
1	A	48	GLN
1	A	140	GLN
1	A	236	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 [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

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	1.58	1 (10%)	14,14,14	0.83	1 (7%)
2	XYP	D	501	-	10,10,10	1.56	1 (10%)	14,14,14	0.72	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	-	-	-	0/1/1/1
2	XYP	D	501	-	-	-	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	O5-C1	-4.51	1.35	1.43
2	D	501	XYP	O5-C1	-4.34	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	XYP	C5-C4-C3	2.84	113.78	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	305/311 (98%)	-0.59	0 100 100	12, 34, 58, 82	1 (0%)
1	B	305/311 (98%)	-0.59	0 100 100	14, 34, 59, 82	1 (0%)
1	C	305/311 (98%)	-0.41	0 100 100	19, 40, 71, 108	1 (0%)
1	D	305/311 (98%)	-0.43	0 100 100	20, 40, 73, 105	0
All	All	1220/1244 (98%)	-0.50	0 100 100	12, 37, 66, 108	3 (0%)

There are no RSRZ outliers to report.

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
2	XYP	C	500	10/10	0.96	0.07	15,35,47,58	0
2	XYP	D	501	10/10	0.97	0.06	17,34,41,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.