



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 11:25 AM JST

PDB ID : 5Z1B
Title : Structure of Bifidobacterium dentium beta-glucuronidase complexed with coumarin-3-O-glucuronide
Authors : Dashnyam, P.; Lin, H.Y.; Lin, C.H.
Deposited on : 2017-12-25
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

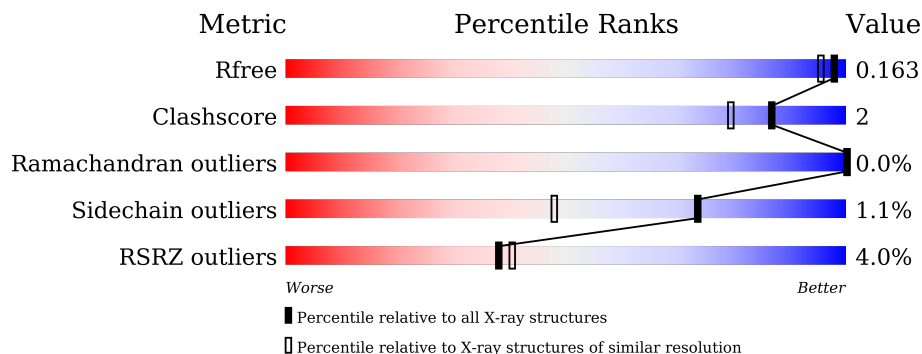
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	692	 4% 85% 5% 9%
1	B	692	 5% 85% 10%
1	C	692	 2% 85% 5% 10%
1	D	692	 4% 85% 5% 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SE2	B	702	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22105 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 Glycosyl hydrolase family 2, TIM barrel domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	627	4948	3134	863	932	19	0	0	0
1	B	620	4905	3111	856	919	19	0	0	0
1	C	624	4927	3123	860	925	19	0	0	0
1	D	622	4916	3117	858	922	19	0	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP E0QAF3
A	-22	HIS	-	expression tag	UNP E0QAF3
A	-21	HIS	-	expression tag	UNP E0QAF3
A	-20	HIS	-	expression tag	UNP E0QAF3
A	-19	HIS	-	expression tag	UNP E0QAF3
A	-18	HIS	-	expression tag	UNP E0QAF3
A	-17	HIS	-	expression tag	UNP E0QAF3
A	-16	SER	-	expression tag	UNP E0QAF3
A	-15	SER	-	expression tag	UNP E0QAF3
A	-14	GLY	-	expression tag	UNP E0QAF3
A	-13	VAL	-	expression tag	UNP E0QAF3
A	-12	ASP	-	expression tag	UNP E0QAF3
A	-11	LEU	-	expression tag	UNP E0QAF3
A	-10	GLY	-	expression tag	UNP E0QAF3
A	-9	THR	-	expression tag	UNP E0QAF3
A	-8	GLU	-	expression tag	UNP E0QAF3
A	-7	ASN	-	expression tag	UNP E0QAF3
A	-6	LEU	-	expression tag	UNP E0QAF3
A	-5	TYR	-	expression tag	UNP E0QAF3
A	-4	PHE	-	expression tag	UNP E0QAF3
A	-3	GLN	-	expression tag	UNP E0QAF3

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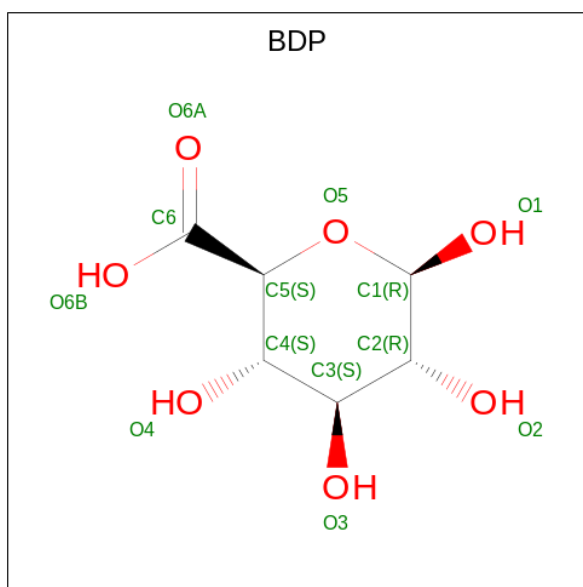
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP E0QAF3
A	-1	ASN	-	expression tag	UNP E0QAF3
A	0	GLY	-	expression tag	UNP E0QAF3
A	479	ALA	GLU	engineered mutation	UNP E0QAF3
B	-23	MET	-	initiating methionine	UNP E0QAF3
B	-22	HIS	-	expression tag	UNP E0QAF3
B	-21	HIS	-	expression tag	UNP E0QAF3
B	-20	HIS	-	expression tag	UNP E0QAF3
B	-19	HIS	-	expression tag	UNP E0QAF3
B	-18	HIS	-	expression tag	UNP E0QAF3
B	-17	HIS	-	expression tag	UNP E0QAF3
B	-16	SER	-	expression tag	UNP E0QAF3
B	-15	SER	-	expression tag	UNP E0QAF3
B	-14	GLY	-	expression tag	UNP E0QAF3
B	-13	VAL	-	expression tag	UNP E0QAF3
B	-12	ASP	-	expression tag	UNP E0QAF3
B	-11	LEU	-	expression tag	UNP E0QAF3
B	-10	GLY	-	expression tag	UNP E0QAF3
B	-9	THR	-	expression tag	UNP E0QAF3
B	-8	GLU	-	expression tag	UNP E0QAF3
B	-7	ASN	-	expression tag	UNP E0QAF3
B	-6	LEU	-	expression tag	UNP E0QAF3
B	-5	TYR	-	expression tag	UNP E0QAF3
B	-4	PHE	-	expression tag	UNP E0QAF3
B	-3	GLN	-	expression tag	UNP E0QAF3
B	-2	SER	-	expression tag	UNP E0QAF3
B	-1	ASN	-	expression tag	UNP E0QAF3
B	0	GLY	-	expression tag	UNP E0QAF3
B	479	ALA	GLU	engineered mutation	UNP E0QAF3
C	-23	MET	-	initiating methionine	UNP E0QAF3
C	-22	HIS	-	expression tag	UNP E0QAF3
C	-21	HIS	-	expression tag	UNP E0QAF3
C	-20	HIS	-	expression tag	UNP E0QAF3
C	-19	HIS	-	expression tag	UNP E0QAF3
C	-18	HIS	-	expression tag	UNP E0QAF3
C	-17	HIS	-	expression tag	UNP E0QAF3
C	-16	SER	-	expression tag	UNP E0QAF3
C	-15	SER	-	expression tag	UNP E0QAF3
C	-14	GLY	-	expression tag	UNP E0QAF3
C	-13	VAL	-	expression tag	UNP E0QAF3
C	-12	ASP	-	expression tag	UNP E0QAF3
C	-11	LEU	-	expression tag	UNP E0QAF3

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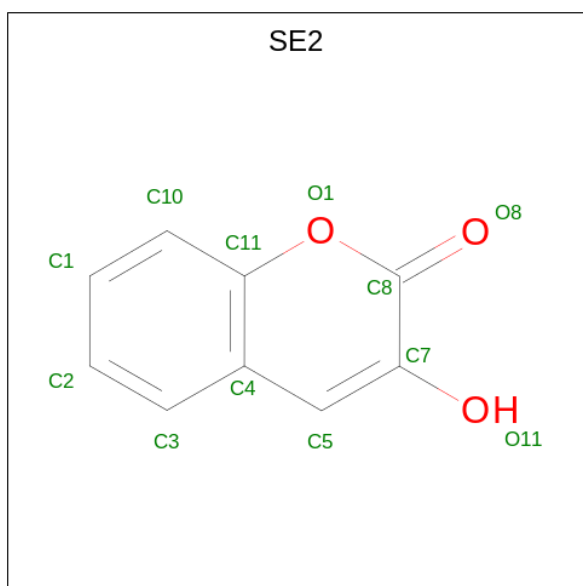
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	expression tag	UNP E0QAF3
C	-9	THR	-	expression tag	UNP E0QAF3
C	-8	GLU	-	expression tag	UNP E0QAF3
C	-7	ASN	-	expression tag	UNP E0QAF3
C	-6	LEU	-	expression tag	UNP E0QAF3
C	-5	TYR	-	expression tag	UNP E0QAF3
C	-4	PHE	-	expression tag	UNP E0QAF3
C	-3	GLN	-	expression tag	UNP E0QAF3
C	-2	SER	-	expression tag	UNP E0QAF3
C	-1	ASN	-	expression tag	UNP E0QAF3
C	0	GLY	-	expression tag	UNP E0QAF3
C	479	ALA	GLU	engineered mutation	UNP E0QAF3
D	-23	MET	-	initiating methionine	UNP E0QAF3
D	-22	HIS	-	expression tag	UNP E0QAF3
D	-21	HIS	-	expression tag	UNP E0QAF3
D	-20	HIS	-	expression tag	UNP E0QAF3
D	-19	HIS	-	expression tag	UNP E0QAF3
D	-18	HIS	-	expression tag	UNP E0QAF3
D	-17	HIS	-	expression tag	UNP E0QAF3
D	-16	SER	-	expression tag	UNP E0QAF3
D	-15	SER	-	expression tag	UNP E0QAF3
D	-14	GLY	-	expression tag	UNP E0QAF3
D	-13	VAL	-	expression tag	UNP E0QAF3
D	-12	ASP	-	expression tag	UNP E0QAF3
D	-11	LEU	-	expression tag	UNP E0QAF3
D	-10	GLY	-	expression tag	UNP E0QAF3
D	-9	THR	-	expression tag	UNP E0QAF3
D	-8	GLU	-	expression tag	UNP E0QAF3
D	-7	ASN	-	expression tag	UNP E0QAF3
D	-6	LEU	-	expression tag	UNP E0QAF3
D	-5	TYR	-	expression tag	UNP E0QAF3
D	-4	PHE	-	expression tag	UNP E0QAF3
D	-3	GLN	-	expression tag	UNP E0QAF3
D	-2	SER	-	expression tag	UNP E0QAF3
D	-1	ASN	-	expression tag	UNP E0QAF3
D	0	GLY	-	expression tag	UNP E0QAF3
D	479	ALA	GLU	engineered mutation	UNP E0QAF3

- Molecule 2 is beta-D-glucopyranuronic acid (three-letter code: BDP) (formula: C₆H₁₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

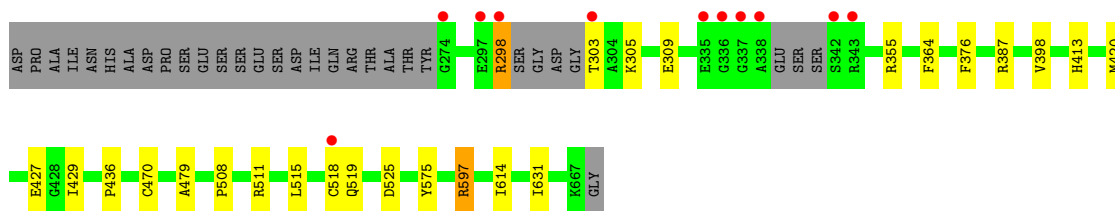
- Molecule 3 is 3-HYDROXY-2H-CHROMEN-2-ONE (three-letter code: SE2) (formula: $C_9H_6O_3$).



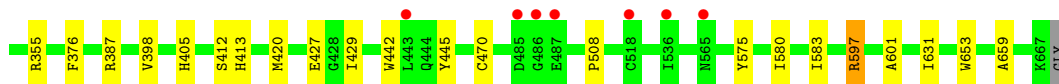
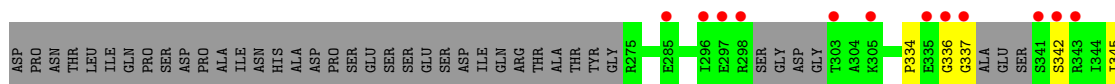
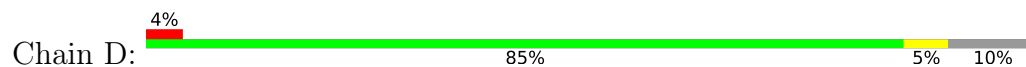
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	9	3		
3	B	1	Total	C	O	0	0
			12	9	3		
3	C	1	Total	C	O	0	0
			12	9	3		
3	D	1	Total	C	O	0	0
			12	9	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	652	Total	O	0	0
			652	652		
4	B	502	Total	O	0	0
			502	502		
4	C	626	Total	O	0	0
			626	626		
4	D	533	Total	O	0	0
			533	533		



● Molecule 1: Glycosyl hydrolase family 2, TIM barrel domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.34Å 104.17Å 160.67Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	29.16 – 1.45 29.16 – 1.45	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.16-1.45) 94.2 (29.16-1.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.45Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.130 , 0.160 0.136 , 0.163	Depositor DCC
R_{free} test set	2002 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22105	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BDP, SE2

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	0.66	0/5080	0.76	4/6912 (0.1%)
1	B	0.56	0/5036	0.69	7/6852 (0.1%)
1	C	0.64	0/5058	0.75	5/6881 (0.1%)
1	D	0.56	0/5047	0.68	3/6866 (0.0%)
All	All	0.61	0/20221	0.72	19/27511 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	A	387	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	C	387	ARG	NE-CZ-NH2	-11.21	114.70	120.30
1	A	387	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	D	387	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	D	387	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	355	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	387	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	387	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	355	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	518	CYS	CA-CB-SG	6.11	124.99	114.00
1	C	597	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	459	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	511	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	597	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	597	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	525	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	597	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	78	LEU	CA-CB-CG	5.08	126.99	115.30

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	4948	0	4692	23	0
1	B	4905	0	4658	23	0
1	C	4927	0	4675	23	0
1	D	4916	0	4668	19	0
2	A	12	0	7	0	0
2	B	12	0	7	0	0
2	C	12	0	7	0	0
2	D	12	0	7	0	0
3	A	12	0	5	3	0
3	B	12	0	5	5	0
3	C	12	0	5	2	0
3	D	12	0	5	2	0
4	A	652	0	0	0	0
4	B	502	0	0	0	0
4	C	626	0	0	1	1
4	D	533	0	0	1	0
All	All	22105	0	18741	81	1

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 2.

All (81) 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:231:THR:OG1	1:A:305:LYS:NZ	2.07	0.87
1:B:235:ASP:OD2	1:B:298:ARG:NH2	2.20	0.75
1:D:153:MET:HE1	3:D:702:SE2:H3	1.67	0.75
1:D:336:GLY:H	1:D:337:GLY:HA3	1.54	0.72
1:C:298:ARG:CZ	1:C:303:THR:HB	2.24	0.68
1:D:75:PRO:HB2	1:D:78:LEU:HD13	1.76	0.68
1:D:336:GLY:N	1:D:337:GLY:HA3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:CE	3:A:702:SE2:H3	2.27	0.65
1:B:518:CYS:SG	3:B:702:SE2:C8	2.85	0.64
1:B:26:GLU:OE1	1:B:172:ARG:NE	2.32	0.61
1:B:153:MET:CE	3:B:702:SE2:H3	2.30	0.61
1:A:153:MET:HE2	3:A:702:SE2:H3	1.84	0.59
1:B:26:GLU:OE1	1:B:172:ARG:NH2	2.35	0.58
1:B:229:ASP:OD2	1:B:305:LYS:HE2	2.03	0.58
1:C:479:ALA:CB	1:C:518:CYS:HB2	2.33	0.58
1:C:229:ASP:CG	1:C:305:LYS:HZ2	2.07	0.57
1:A:631:ILE:HG22	1:B:631:ILE:HG22	1.87	0.55
1:B:479:ALA:CB	1:B:518:CYS:HB2	2.37	0.54
1:A:78:LEU:HD12	1:C:78:LEU:HD13	1.89	0.54
1:B:355:ARG:NH1	1:B:355:ARG:O	2.40	0.54
1:B:153:MET:HE1	3:B:702:SE2:H3	1.90	0.53
1:C:631:ILE:HG22	1:D:631:ILE:HG22	1.89	0.53
1:C:207:THR:HG21	1:C:508:PRO:HB2	1.91	0.52
1:B:278:ARG:NH1	1:B:293:THR:OG1	2.40	0.52
1:D:172:ARG:NH1	4:D:802:HOH:O	2.43	0.51
1:C:398:VAL:HG11	1:C:427:GLU:HG3	1.93	0.51
1:C:102:GLN:NE2	4:C:804:HOH:O	2.43	0.50
1:B:153:MET:HB3	1:B:631:ILE:HD11	1.94	0.50
1:A:316:LYS:HD2	1:A:324:TYR:CZ	2.47	0.49
1:A:13:PHE:CE1	1:C:11:ILE:HD11	2.48	0.48
3:A:702:SE2:H1	1:B:157:ASN:HD21	1.78	0.48
1:B:398:VAL:HG11	1:B:427:GLU:HG3	1.94	0.48
1:D:398:VAL:HG11	1:D:427:GLU:HG3	1.96	0.48
1:B:355:ARG:HH11	1:B:355:ARG:C	2.17	0.47
1:A:316:LYS:HD2	1:A:324:TYR:CE2	2.50	0.47
3:C:702:SE2:H1	1:D:157:ASN:HD21	1.80	0.46
1:A:157:ASN:HD21	3:B:702:SE2:H1	1.80	0.46
1:B:153:MET:HE3	3:B:702:SE2:H3	1.97	0.46
1:A:78:LEU:HA	1:C:78:LEU:HD21	1.97	0.46
1:C:479:ALA:HB1	1:C:518:CYS:HB2	1.97	0.46
1:A:13:PHE:CD1	1:C:11:ILE:HD11	2.52	0.45
1:A:398:VAL:HG11	1:A:427:GLU:HG3	1.99	0.45
1:D:123:HIS:HE1	1:D:126:GLU:O	1.99	0.45
1:D:405:HIS:CD2	1:D:659:ALA:HB2	2.51	0.45
1:B:92:THR:HA	1:B:93:HIS:HA	1.82	0.45
1:C:229:ASP:OD2	1:C:305:LYS:NZ	2.50	0.44
1:B:26:GLU:OE1	1:B:172:ARG:CZ	2.65	0.44
1:C:305:LYS:HB3	1:C:305:LYS:HE3	1.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ARG:HA	1:B:343:ARG:HD2	1.66	0.43
1:D:429:ILE:O	1:D:470:CYS:HB2	2.18	0.43
1:D:442:TRP:HA	1:D:445:TYR:CD2	2.53	0.43
1:A:479:ALA:CB	1:A:518:CYS:HB2	2.48	0.43
1:D:336:GLY:H	1:D:337:GLY:CA	2.27	0.43
1:D:580:ILE:HB	1:D:583:ILE:HD12	2.00	0.43
1:A:11:ILE:HD11	1:C:13:PHE:CD1	2.54	0.43
1:C:429:ILE:O	1:C:470:CYS:HB2	2.19	0.42
1:D:334:PRO:HB3	1:D:345:ILE:HD11	2.01	0.42
1:B:330:ALA:O	1:B:347:ALA:HA	2.19	0.42
1:D:92:THR:HA	1:D:93:HIS:HA	1.85	0.42
1:A:207:THR:HG21	1:A:508:PRO:HB2	2.01	0.42
1:A:429:ILE:O	1:A:470:CYS:HB2	2.19	0.42
1:B:395:VAL:HA	1:B:423:LEU:HD21	2.01	0.42
1:C:518:CYS:SG	3:C:702:SE2:C8	3.07	0.41
1:C:515:LEU:C	1:C:515:LEU:HD23	2.41	0.41
1:C:225:LEU:HD11	1:C:309:GLU:HB3	2.02	0.41
1:D:207:THR:HG21	1:D:508:PRO:HB2	2.03	0.41
1:C:157:ASN:HD21	3:D:702:SE2:H1	1.85	0.41
1:C:364:PHE:HB2	1:C:614:ILE:HD13	2.02	0.41
1:D:412:SER:HA	1:D:413:HIS:HA	1.84	0.41
1:A:412:SER:HA	1:A:413:HIS:HA	1.86	0.41
1:A:442:TRP:HA	1:A:445:TYR:CD2	2.56	0.41
1:A:601:ALA:HA	1:A:653:TRP:CH2	2.55	0.41
1:B:479:ALA:HB1	1:B:518:CYS:HB2	2.02	0.41
1:C:518:CYS:O	1:C:519:GLN:C	2.59	0.41
1:A:364:PHE:HB2	1:A:614:ILE:HD13	2.02	0.40
1:A:225:LEU:HD11	1:A:309:GLU:HB3	2.03	0.40
1:A:580:ILE:HB	1:A:583:ILE:HD12	2.03	0.40
1:A:153:MET:HB3	1:A:631:ILE:HD11	2.03	0.40
1:B:580:ILE:HB	1:B:583:ILE:HD12	2.03	0.40
1:C:413:HIS:O	1:C:436:PRO:HA	2.21	0.40
1:D:601:ALA:HA	1:D:653:TRP:CH2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1244:HOH:O	4:C:1418:HOH:O[2_454]	2.18	0.02

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	621/692 (90%)	600 (97%)	21 (3%)	0	100	100
1	B	612/692 (88%)	592 (97%)	20 (3%)	0	100	100
1	C	616/692 (89%)	595 (97%)	21 (3%)	0	100	100
1	D	614/692 (89%)	591 (96%)	22 (4%)	1 (0%)	47	22
All	All	2463/2768 (89%)	2378 (96%)	84 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	342	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	506/563 (90%)	500 (99%)	6 (1%)	71	43
1	B	502/563 (89%)	497 (99%)	5 (1%)	76	52
1	C	503/563 (89%)	497 (99%)	6 (1%)	71	43
1	D	503/563 (89%)	497 (99%)	6 (1%)	71	43
All	All	2014/2252 (89%)	1991 (99%)	23 (1%)	73	48

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ARG
1	A	376	PHE
1	A	420	MET
1	A	569	PRO
1	A	575	TYR
1	A	597	ARG
1	B	355	ARG
1	B	376	PHE
1	B	420	MET
1	B	575	TYR
1	B	597	ARG
1	C	298	ARG
1	C	355	ARG
1	C	376	PHE
1	C	420	MET
1	C	575	TYR
1	C	597	ARG
1	D	153	MET
1	D	355	ARG
1	D	376	PHE
1	D	420	MET
1	D	575	TYR
1	D	597	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	-1	ASN
1	C	82	GLN
1	C	102	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	SE2	A	702	2	13,13,13	2.88	6 (46%)	14,18,18	1.92	6 (42%)
2	BDP	B	701	3	12,12,13	1.54	2 (16%)	14,17,19	1.84	4 (28%)
3	SE2	C	702	2	13,13,13	3.12	6 (46%)	14,18,18	2.18	5 (35%)
2	BDP	A	701	3	12,12,13	1.70	4 (33%)	14,17,19	1.92	2 (14%)
3	SE2	B	702	2	13,13,13	3.37	5 (38%)	14,18,18	1.22	2 (14%)
2	BDP	D	701	3	12,12,13	1.71	3 (25%)	14,17,19	1.85	3 (21%)
2	BDP	C	701	3	12,12,13	1.94	3 (25%)	14,17,19	1.44	1 (7%)
3	SE2	D	702	2	13,13,13	3.28	5 (38%)	14,18,18	1.38	2 (14%)

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
3	SE2	A	702	2	-	-	0/2/2/2
2	BDP	B	701	3	-	0/4/21/24	0/1/1/1
3	SE2	C	702	2	-	-	0/2/2/2
2	BDP	A	701	3	-	1/4/21/24	0/1/1/1
3	SE2	B	702	2	-	-	0/2/2/2
2	BDP	D	701	3	-	0/4/21/24	0/1/1/1
2	BDP	C	701	3	-	0/4/21/24	0/1/1/1
3	SE2	D	702	2	-	-	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	SE2	O1-C11	7.81	1.50	1.38
3	D	702	SE2	O1-C11	6.84	1.49	1.38
3	D	702	SE2	C5-C7	6.10	1.48	1.37
3	B	702	SE2	C5-C7	6.05	1.48	1.37
3	C	702	SE2	C5-C7	5.99	1.48	1.37
3	A	702	SE2	C5-C7	5.81	1.48	1.37
3	C	702	SE2	O1-C11	5.22	1.46	1.38
3	A	702	SE2	O1-C11	4.77	1.45	1.38
3	C	702	SE2	O11-C7	4.46	1.45	1.34
3	D	702	SE2	O1-C8	4.28	1.43	1.38
3	A	702	SE2	C4-C5	4.23	1.52	1.43
3	D	702	SE2	C4-C5	4.15	1.52	1.43
3	B	702	SE2	C4-C5	4.03	1.52	1.43
3	C	702	SE2	O1-C8	3.95	1.43	1.38
3	C	702	SE2	C4-C5	3.93	1.51	1.43
3	A	702	SE2	O11-C7	3.91	1.44	1.34
3	B	702	SE2	O1-C8	3.76	1.43	1.38
3	D	702	SE2	O11-C7	3.72	1.43	1.34
3	B	702	SE2	O11-C7	3.49	1.43	1.34
2	D	701	BDP	C2-C3	-3.46	1.47	1.52
2	B	701	BDP	C2-C3	-3.33	1.47	1.52
2	C	701	BDP	C2-C3	-3.27	1.47	1.52
3	A	702	SE2	O1-C8	3.23	1.42	1.38
2	C	701	BDP	O6B-C6	-3.10	1.20	1.30
2	A	701	BDP	O5-C5	2.87	1.48	1.43
2	A	701	BDP	C2-C3	-2.84	1.48	1.52
2	C	701	BDP	O5-C5	2.78	1.48	1.43
3	C	702	SE2	C7-C8	2.63	1.52	1.46
2	A	701	BDP	O6B-C6	-2.37	1.22	1.30
2	D	701	BDP	O5-C5	2.37	1.47	1.43
3	A	702	SE2	C7-C8	2.33	1.51	1.46
2	B	701	BDP	O5-C5	2.31	1.47	1.43
2	D	701	BDP	C4-C3	-2.17	1.46	1.52
2	A	701	BDP	C5-C6	-2.01	1.48	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	BDP	C1-C2-C3	6.02	117.07	109.67
2	D	701	BDP	C1-C2-C3	4.94	115.74	109.67
3	C	702	SE2	O1-C8-O8	-4.94	109.69	116.22
2	B	701	BDP	C1-C2-C3	4.64	115.37	109.67
2	C	701	BDP	C1-C2-C3	4.37	115.04	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	SE2	C11-C4-C5	4.07	121.20	118.04
3	A	702	SE2	O1-C8-O8	-4.02	110.90	116.22
3	D	702	SE2	C11-C4-C5	3.25	120.57	118.04
2	D	701	BDP	O6B-C6-C5	3.24	125.53	113.65
2	B	701	BDP	O6B-C6-C5	3.13	125.12	113.65
3	A	702	SE2	O8-C8-C7	2.86	129.37	125.14
2	A	701	BDP	C3-C4-C5	-2.86	104.36	109.25
3	A	702	SE2	C11-C4-C5	2.68	120.13	118.04
2	B	701	BDP	O4-C4-C3	2.52	116.18	110.35
3	B	702	SE2	O1-C11-C10	2.46	119.52	116.26
3	D	702	SE2	O1-C11-C10	2.46	119.51	116.26
3	B	702	SE2	C11-C4-C5	2.44	119.94	118.04
3	C	702	SE2	O8-C8-C7	2.33	128.58	125.14
3	C	702	SE2	C10-C11-C4	2.28	122.15	118.17
2	D	701	BDP	O6A-C6-C5	-2.22	112.68	120.81
3	A	702	SE2	O1-C11-C10	2.19	119.17	116.26
2	B	701	BDP	O6A-C6-C5	-2.18	112.83	120.81
3	A	702	SE2	O11-C7-C5	-2.17	115.49	121.48
3	A	702	SE2	C10-C11-C4	2.15	121.93	118.17
3	C	702	SE2	C11-O1-C8	-2.10	120.19	122.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	BDP	O5-C5-C6-O6B

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	SE2	3	0
3	C	702	SE2	2	0
3	B	702	SE2	5	0
3	D	702	SE2	2	0

5.7 Other polymers [i](#)

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	627/692 (90%)	-0.38	25 (3%) 38 40	7, 12, 31, 62	0
1	B	620/692 (89%)	-0.04	32 (5%) 27 30	10, 23, 43, 85	0
1	C	624/692 (90%)	-0.40	14 (2%) 62 65	8, 14, 32, 74	0
1	D	622/692 (89%)	-0.13	29 (4%) 31 34	10, 23, 43, 81	0
All	All	2493/2768 (90%)	-0.24	100 (4%) 38 40	7, 18, 40, 85	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	303	THR	8.8
1	C	338	ALA	8.6
1	D	336	GLY	8.1
1	B	342	SER	6.7
1	A	340	SER	6.4
1	B	518	CYS	6.3
1	B	274	GLY	6.2
1	B	343	ARG	6.1
1	B	298	ARG	6.0
1	B	303	THR	5.5
1	D	298	ARG	5.3
1	A	303	THR	5.2
1	D	-1	ASN	5.0
1	C	518	CYS	4.9
1	D	341	SER	4.9
1	C	337	GLY	4.9
1	B	235	ASP	4.9
1	D	343	ARG	4.7
1	C	342	SER	4.7
1	D	234	GLY	4.6
1	C	336	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	4.4
1	A	343	ARG	4.3
1	C	343	ARG	4.3
1	A	338	ALA	4.2
1	A	342	SER	4.1
1	D	335	GLU	4.1
1	B	78	LEU	4.0
1	A	337	GLY	4.0
1	C	335	GLU	4.0
1	A	341	SER	3.9
1	C	298	ARG	3.8
1	D	148	ALA	3.7
1	B	153	MET	3.6
1	D	342	SER	3.6
1	D	297	GLU	3.6
1	D	487	GLU	3.6
1	B	124	ALA	3.6
1	B	297	GLU	3.6
1	D	303	THR	3.6
1	A	298	ARG	3.5
1	B	152	PHE	3.4
1	A	518	CYS	3.4
1	A	339	GLU	3.4
1	D	198	ASP	3.3
1	D	305	LYS	3.3
1	B	198	ASP	3.2
1	A	148	ALA	3.2
1	B	-1	ASN	3.1
1	D	78	LEU	3.1
1	B	213	HIS	3.0
1	C	235	ASP	3.0
1	A	153	MET	3.0
1	D	486	GLY	3.0
1	C	297	GLU	2.9
1	B	275	ARG	2.9
1	B	214	ILE	2.9
1	A	336	GLY	2.8
1	A	152	PHE	2.8
1	D	536	ILE	2.8
1	B	234	GLY	2.8
1	B	13	PHE	2.7
1	A	78	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	297	GLU	2.7
1	B	148	ALA	2.7
1	B	296	ILE	2.7
1	D	153	MET	2.7
1	C	148	ALA	2.5
1	A	169	HIS	2.5
1	B	565	ASN	2.5
1	D	518	CYS	2.5
1	A	159	ASN	2.4
1	B	216	GLY	2.4
1	A	335	GLU	2.4
1	B	487	GLU	2.3
1	A	274	GLY	2.3
1	A	151	ALA	2.3
1	A	154	GLY	2.3
1	D	337	GLY	2.3
1	B	76	SER	2.3
1	B	77	ARG	2.3
1	D	81	GLY	2.3
1	D	149	GLY	2.3
1	B	334	PRO	2.2
1	D	485	ASP	2.2
1	C	169	HIS	2.2
1	D	443	LEU	2.2
1	D	77	ARG	2.2
1	C	274	GLY	2.2
1	D	285	GLU	2.2
1	B	79	VAL	2.2
1	B	151	ALA	2.1
1	B	293	THR	2.1
1	A	150	THR	2.1
1	D	124	ALA	2.1
1	A	334	PRO	2.1
1	B	37	PRO	2.1
1	D	565	ASN	2.1
1	B	149	GLY	2.0
1	D	296	ILE	2.0

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SE2	C	702	12/12	0.75	0.20	28,31,33,33	0
3	SE2	B	702	12/12	0.79	0.25	34,36,36,37	0
3	SE2	D	702	12/12	0.82	0.22	33,35,36,36	0
3	SE2	A	702	12/12	0.87	0.17	25,27,28,28	0
2	BDP	D	701	12/13	0.93	0.11	18,24,29,30	0
2	BDP	C	701	12/13	0.94	0.11	14,19,25,25	0
2	BDP	B	701	12/13	0.94	0.10	15,22,28,30	0
2	BDP	A	701	12/13	0.95	0.11	12,17,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.