Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 05:34 AM EDT

PDB ID	:	3RU4
Title	:	Crystal structure of the Bowman-Birk serine protease inhibitor BTCI in complex with trypsin and chymotrypsin
Authors	:	Esteves, G.F.; Santos, C.R.; Ventura, M.M.; Barbosa, J.A.R.G.; Freitas, S.M.
Deposited on	:	2011-05-04
Resolution	:	1.68 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 (i) 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 (i)) were used in the production of this report:

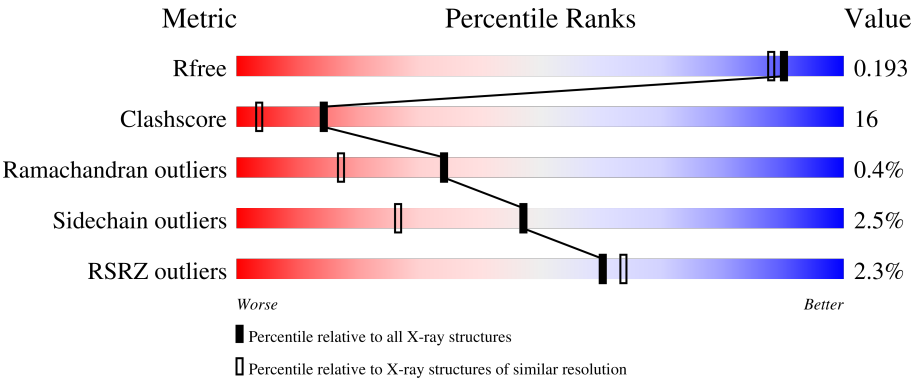
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 <=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	T	223	74% 24%
2	B	61	7% 77% 18% 5%
3	C	11	9% 91% 9%
4	D	131	2% 84% 16%
5	E	96	3% 83% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MRD	T	242	-	-	X	-
7	GOL	T	4	-	X	X	-
7	GOL	T	5	-	-	X	-
8	SO4	B	12	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4732 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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	223	Total	C	N	O	S	0	6	0
			1654	1031	280	329	14			

- Molecule 2 is a protein called Bowman-Birk type seed trypsin and chymotrypsin inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	61	Total	C	N	O	S	0	3	0
			470	284	84	88	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ASP	ARG	conflict	UNP P17734
B	21	ARG	GLU	conflict	UNP P17734
B	23	GLU	ALA	conflict	UNP P17734
B	36	ASP	GLU	conflict	UNP P17734

- Molecule 3 is a protein called Chymotrypsinogen A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	S	0	0	0
			75	48	12	14	1			

- Molecule 4 is a protein called Chymotrypsinogen A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	131	Total	C	N	O	S	0	8	0
			1011	643	163	201	4			

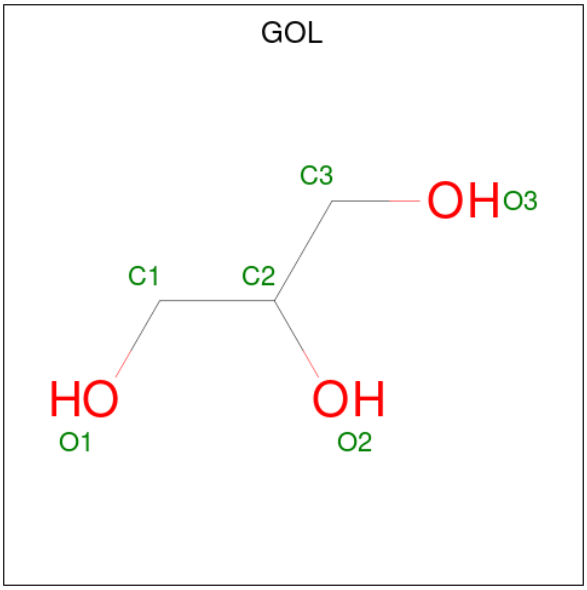
- Molecule 5 is a protein called Chymotrypsinogen A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	96	Total	C	N	O	S	0	2	0
			706	439	123	137	7			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

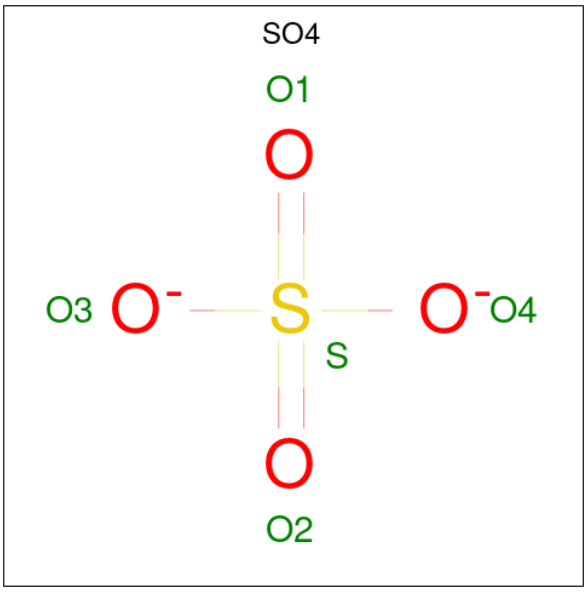
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	1	Total	Ca	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



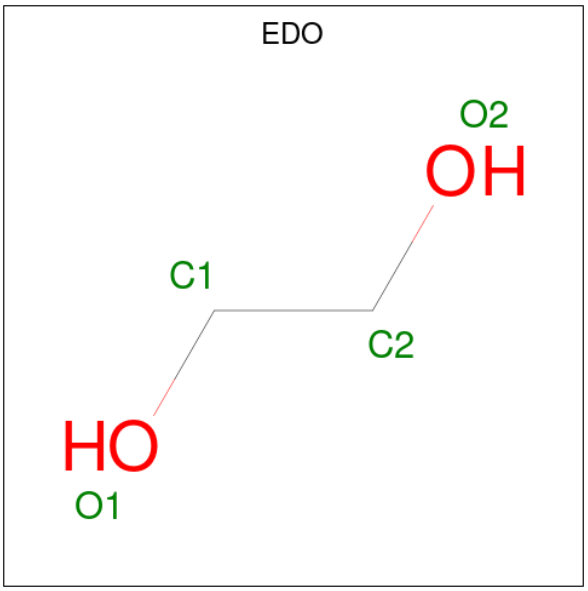
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	T	1	Total	C	O	0	0
			6	3	3		
7	T	1	Total	C	O	0	0
			6	3	3		
7	T	1	Total	C	O	0	0
			6	3	3		
7	T	1	Total	C	O	0	0
			6	3	3		
7	T	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



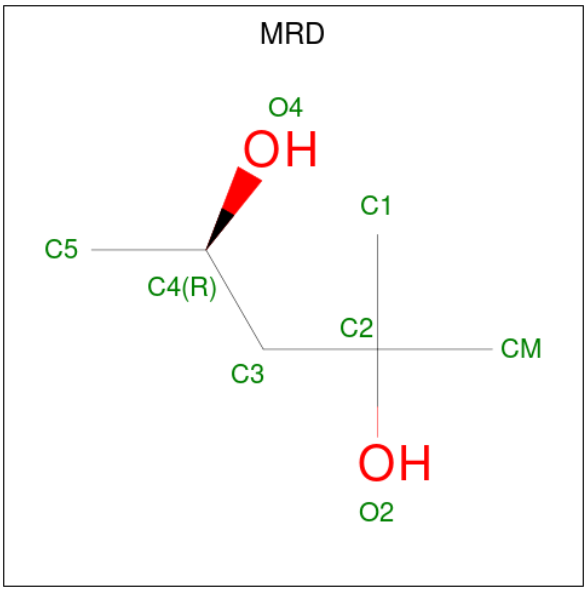
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	T	1	Total O S 5 4 1	0	0
8	T	1	Total O S 5 4 1	0	0
8	T	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0
8	E	1	Total O S 5 4 1	0	0
8	E	1	Total O S 5 4 1	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	T	1	Total	C	O	0	0
			4	2	2		
9	T	1	Total	C	O	0	0
			4	2	2		
9	T	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	T	1	Total C O 8 6 2	0	0
10	D	1	Total C O 8 6 2	0	0

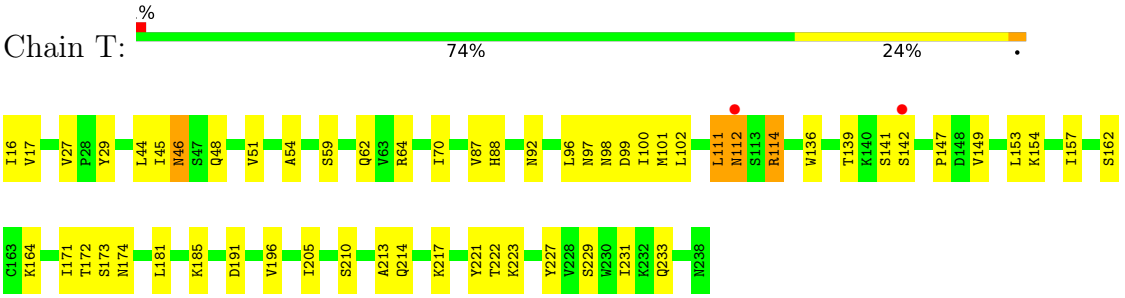
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	T	319	Total O 319 319	0	0
11	B	88	Total O 88 88	0	0
11	C	12	Total O 12 12	0	0
11	D	174	Total O 174 174	0	0
11	E	101	Total O 101 101	0	0

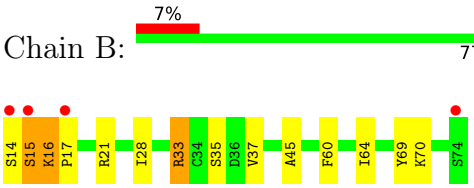
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

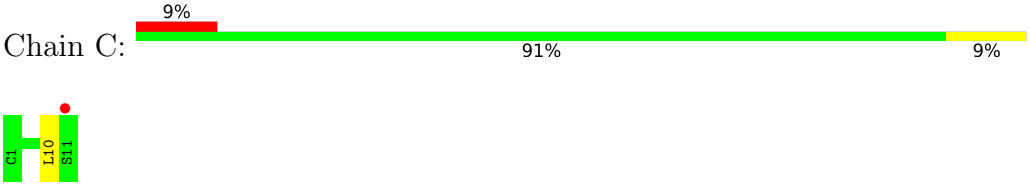
• Molecule 1: Cationic trypsin



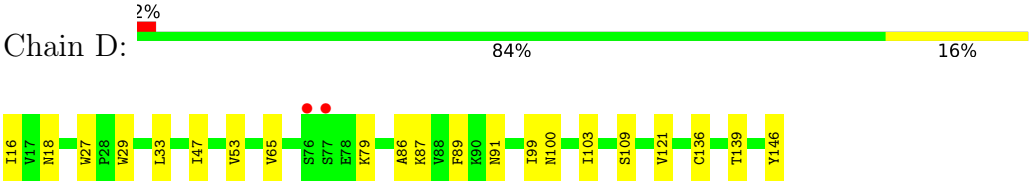
• Molecule 2: Bowman-Birk type seed trypsin and chymotrypsin inhibitor



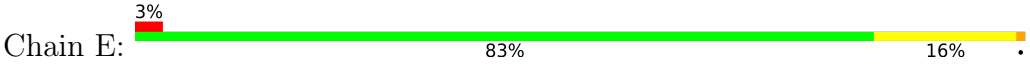
• Molecule 3: Chymotrypsinogen A

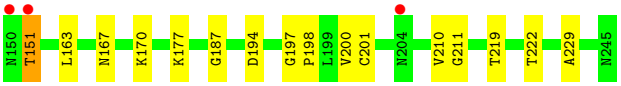


• Molecule 4: Chymotrypsinogen A



• Molecule 5: Chymotrypsinogen A




N150
T151
L163
N167
K170
K177
G187
D194
G197
P198
L199
V200
C201
N204
V210
G211
T219
T222
A229
N245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.48Å 54.57Å 69.29Å 67.28° 71.04° 73.55°	Depositor
Resolution (Å)	62.02 – 1.68 19.56 – 1.68	Depositor EDS
% Data completeness (in resolution range)	80.2 (62.02-1.68) 80.3 (19.56-1.68)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.157 , 0.192 0.158 , 0.193	Depositor DCC
R_{free} test set	2899 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4732	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	T	1.03	0/1703	1.05	1/2307 (0.0%)
2	B	1.03	0/491	1.08	0/659
3	C	0.99	0/76	0.88	0/103
4	D	0.98	0/1055	0.97	1/1437 (0.1%)
5	E	1.02	0/725	1.00	0/987
All	All	1.02	0/4050	1.02	2/5493 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	154	LYS	CD-CE-NZ	-6.27	97.27	111.70
4	D	136	CYS	CA-CB-SG	-5.04	104.93	114.00

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	T	1654	0	1631	56	0
2	B	470	0	440	37	0
3	C	75	0	81	0	0
4	D	1011	0	1008	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	706	0	706	17	0
6	T	1	0	0	0	0
7	B	6	0	8	0	0
7	T	30	0	40	12	0
8	B	10	0	0	5	0
8	D	10	0	0	0	0
8	E	10	0	0	0	0
8	T	15	0	0	1	0
9	D	4	0	6	2	0
9	E	8	0	12	1	0
9	T	12	0	18	3	0
10	D	8	0	14	0	0
10	T	8	0	14	6	0
11	B	88	0	0	3	0
11	C	12	0	0	0	0
11	D	174	0	0	4	0
11	E	101	0	0	6	0
11	T	319	0	0	5	1
All	All	4732	0	3978	124	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 16.

All (124) 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)
2:B:16:LYS:CG	2:B:17:PRO:CD	1.76	1.57
2:B:16:LYS:HG3	2:B:17:PRO:CD	1.15	1.54
2:B:16:LYS:CD	2:B:17:PRO:HD3	1.38	1.49
2:B:16:LYS:CG	2:B:17:PRO:HD2	1.34	1.42
2:B:37:VAL:HG22	2:B:60[A]:PHE:CE1	1.65	1.29
2:B:60[A]:PHE:CD2	8:B:12:SO4:O2	1.87	1.26
2:B:16:LYS:CD	2:B:17:PRO:CD	2.06	1.22
2:B:60[A]:PHE:CE2	8:B:12:SO4:O2	1.98	1.16
2:B:16:LYS:HD3	2:B:17:PRO:HD3	1.21	1.10
2:B:16:LYS:CG	2:B:17:PRO:HD3	1.60	1.08
1:T:173:SER:H	7:T:5:GOL:H12	1.14	1.03
4:D:100:ASN:HD22	9:D:147:EDO:H21	1.24	1.01
1:T:92:ASN:HD22	7:T:4:GOL:H2	1.24	1.00
2:B:16:LYS:HD2	2:B:17:PRO:CD	1.98	0.94
2:B:37:VAL:HG22	2:B:60[A]:PHE:HE1	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:CG2	2:B:60[A]:PHE:CE1	2.51	0.93
1:T:54:ALA:HB1	1:T:87[A]:VAL:HG13	1.57	0.87
2:B:16:LYS:HG3	2:B:17:PRO:N	1.90	0.86
2:B:33[B]:ARG:HD3	11:B:609:HOH:O	1.75	0.85
1:T:92:ASN:ND2	7:T:4:GOL:H2	1.95	0.82
1:T:223[B]:LYS:NZ	10:T:242:MRD:H1C2	1.94	0.82
2:B:14:SER:HB2	11:B:648:HOH:O	1.79	0.80
2:B:37:VAL:CG2	2:B:60[A]:PHE:HE1	1.91	0.79
4:D:146:TYR:CD2	5:E:219[A]:THR:HG23	2.19	0.77
2:B:16:LYS:CB	2:B:17:PRO:CD	2.62	0.77
2:B:33[A]:ARG:HG2	2:B:64:ILE:HG12	1.67	0.75
9:E:20:EDO:H22	11:E:510:HOH:O	1.86	0.74
2:B:60[A]:PHE:HD2	8:B:12:SO4:O2	1.69	0.73
2:B:60[A]:PHE:CD2	8:B:12:SO4:S	2.81	0.73
5:E:151:THR:CG2	11:E:637:HOH:O	2.38	0.71
4:D:87:LYS:HE2	11:D:598:HOH:O	1.90	0.71
5:E:151:THR:HG22	11:E:637:HOH:O	1.91	0.70
2:B:33[B]:ARG:CD	11:B:609:HOH:O	2.35	0.69
2:B:17:PRO:HG3	2:B:45:ALA:CB	2.24	0.67
1:T:54:ALA:CB	1:T:87[A]:VAL:HG13	2.24	0.67
1:T:45:ILE:HD13	1:T:51:VAL:HG23	1.77	0.66
1:T:223[B]:LYS:HE3	10:T:242:MRD:H4	1.79	0.65
1:T:62:GLN:HE22	1:T:64:ARG:HH21	1.44	0.65
1:T:173:SER:N	7:T:5:GOL:H12	1.99	0.65
1:T:92:ASN:HD22	7:T:4:GOL:C2	2.07	0.64
1:T:46:ASN:HD22	1:T:48:GLN:H	1.45	0.64
5:E:219[A]:THR:HG22	11:E:515:HOH:O	1.98	0.64
1:T:45:ILE:HD13	1:T:51:VAL:CG2	2.29	0.63
9:D:147:EDO:H11	11:D:649:HOH:O	1.98	0.63
1:T:223[B]:LYS:HZ2	10:T:242:MRD:H1C2	1.61	0.63
2:B:15:SER:HA	2:B:70:LYS:HD3	1.81	0.63
9:T:240:EDO:H21	2:B:28:ILE:HD13	1.80	0.62
1:T:223[B]:LYS:HZ1	10:T:242:MRD:H1C2	1.63	0.62
1:T:46:ASN:HD22	1:T:46:ASN:C	2.03	0.62
1:T:44:LEU:HD21	1:T:111:LEU:HD11	1.83	0.60
5:E:177:LYS:NZ	11:E:634:HOH:O	2.33	0.59
1:T:62:GLN:NE2	1:T:64:ARG:HE	2.01	0.59
2:B:16:LYS:CB	2:B:17:PRO:HD3	2.26	0.59
1:T:174:ASN:HD21	7:T:1:GOL:H2	1.69	0.58
2:B:16:LYS:HG3	2:B:17:PRO:HD2	0.58	0.58
1:T:62:GLN:HE21	1:T:64:ARG:HE	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:PRO:HG3	2:B:45:ALA:HB2	1.85	0.57
1:T:149:VAL:HG22	8:T:8:SO4:O3	2.04	0.57
1:T:46:ASN:ND2	1:T:48:GLN:H	2.03	0.56
1:T:172:THR:HB	7:T:5:GOL:H11	1.87	0.56
1:T:114:ARG:HG3	1:T:114:ARG:NH1	2.21	0.56
1:T:114:ARG:HG3	1:T:114:ARG:HH11	1.71	0.56
10:T:242:MRD:H1C3	11:T:430:HOH:O	2.06	0.55
7:T:6:GOL:H12	11:T:336:HOH:O	2.06	0.54
1:T:97:ASN:ND2	7:T:4:GOL:H12	2.23	0.54
2:B:37:VAL:HG22	2:B:60[A]:PHE:CD1	2.32	0.53
1:T:139:THR:HG23	1:T:147:PRO:HD3	1.91	0.53
1:T:210:SER:O	1:T:217:LYS:HE3	2.08	0.53
1:T:97:ASN:HD22	7:T:4:GOL:H12	1.74	0.53
4:D:87:LYS:HG2	4:D:89:PHE:CE1	2.45	0.52
1:T:54:ALA:HB1	1:T:87[A]:VAL:CG1	2.34	0.52
1:T:157:ILE:HG21	10:T:242:MRD:H3C1	1.91	0.51
1:T:141:SER:HB3	1:T:213:ALA:HB3	1.93	0.50
4:D:86:ALA:HB2	4:D:109:SER:HA	1.93	0.50
5:E:167[B]:ASN:HA	5:E:170:LYS:HD2	1.94	0.49
1:T:233:GLN:HB3	9:T:239:EDO:O2	2.11	0.49
1:T:153:LEU:HD11	1:T:185:LYS:HD3	1.94	0.49
2:B:17:PRO:HG3	2:B:45:ALA:HB3	1.93	0.48
2:B:17:PRO:HG2	2:B:69:TYR:CE2	2.48	0.48
2:B:60[A]:PHE:HD2	8:B:12:SO4:S	2.30	0.48
1:T:172:THR:HB	7:T:5:GOL:C1	2.44	0.48
4:D:47:ILE:HD13	4:D:53[B]:VAL:HG23	1.96	0.47
5:E:187:GLY:C	5:E:222:THR:HB	2.36	0.47
1:T:114:ARG:HH11	1:T:114:ARG:CG	2.28	0.47
11:D:8:HOH:O	5:E:197:GLY:HA3	2.15	0.47
1:T:98:ASN:HA	1:T:227:TYR:OH	2.16	0.46
2:B:16:LYS:HD2	2:B:17:PRO:CG	2.44	0.46
2:B:21:ARG:HD3	2:B:35[A]:SER:OG	2.16	0.45
4:D:29:TRP:CG	4:D:121:VAL:HB	2.51	0.45
5:E:163:LEU:HD23	5:E:167[B]:ASN:ND2	2.31	0.45
1:T:229:SER:OG	7:T:2:GOL:H31	2.17	0.45
1:T:27:VAL:HG13	1:T:29:TYR:CZ	2.51	0.45
1:T:142:SER:HB3	11:T:562:HOH:O	2.15	0.45
1:T:214:GLN:CB	1:T:217:LYS:HE2	2.47	0.45
9:T:239:EDO:H22	11:T:618:HOH:O	2.18	0.44
1:T:98:ASN:ND2	1:T:227:TYR:OH	2.51	0.44
5:E:219[A]:THR:HG21	11:E:267:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:174:ASN:HB3	1:T:227:TYR:HH	1.83	0.44
2:B:33[A]:ARG:CG	2:B:64:ILE:HG12	2.42	0.44
1:T:70:ILE:HG23	1:T:136:TRP:CE2	2.53	0.44
5:E:201:CYS:SG	5:E:210:VAL:HG21	2.58	0.43
1:T:62:GLN:NE2	1:T:64:ARG:HH21	2.15	0.43
1:T:54:ALA:HA	1:T:101:MET:HB2	2.01	0.43
1:T:112:ASN:ND2	11:T:465:HOH:O	2.51	0.43
1:T:88:HIS:HB2	1:T:100:ILE:HG23	2.01	0.43
1:T:164:LYS:HG2	1:T:171:ILE:HB	2.00	0.43
1:T:16:ILE:N	1:T:191:ASP:OD1	2.51	0.42
5:E:198:PRO:HB2	5:E:200:VAL:HG13	2.02	0.42
1:T:162[B]:SER:OG	1:T:181:LEU:HD11	2.20	0.42
1:T:205:ILE:HB	1:T:222:THR:HB	2.03	0.41
2:B:17:PRO:HG2	2:B:69:TYR:CD2	2.55	0.41
1:T:196:VAL:HG21	1:T:221:TYR:CD1	2.56	0.41
5:E:167[A]:ASN:HA	5:E:170:LYS:HD2	2.02	0.41
1:T:102:LEU:HD11	1:T:231:ILE:HA	2.02	0.41
1:T:96:LEU:O	1:T:99:ASP:HB2	2.20	0.41
5:E:211:GLY:HA2	5:E:229:ALA:O	2.21	0.41
4:D:27:TRP:CD1	4:D:139:THR:HG21	2.55	0.41
4:D:91:ASN:HB2	4:D:103:ILE:HG23	2.03	0.41
1:T:17:VAL:O	1:T:185:LYS:HA	2.22	0.40
4:D:65[B]:VAL:HG11	11:D:301:HOH:O	2.20	0.40
4:D:16:ILE:N	5:E:194:ASP:OD1	2.54	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:D:18[B]:ASN:OD1	11:T:376:HOH:O[1_655]	2.19	0.01

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	T	227/223 (102%)	220 (97%)	7 (3%)	0	100 100
2	B	62/61 (102%)	58 (94%)	3 (5%)	1 (2%)	9 1
3	C	9/11 (82%)	9 (100%)	0	0	100 100
4	D	137/131 (105%)	135 (98%)	1 (1%)	1 (1%)	22 8
5	E	96/96 (100%)	92 (96%)	4 (4%)	0	100 100
All	All	531/522 (102%)	514 (97%)	15 (3%)	2 (0%)	34 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	16	LYS
4	D	99	ILE

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	T	190/184 (103%)	185 (97%)	5 (3%)	46 25
2	B	60/57 (105%)	57 (95%)	3 (5%)	24 7
3	C	9/9 (100%)	8 (89%)	1 (11%)	6 1
4	D	117/109 (107%)	114 (97%)	3 (3%)	46 25
5	E	79/77 (103%)	78 (99%)	1 (1%)	69 54
All	All	455/436 (104%)	442 (97%)	13 (3%)	47 21

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	46	ASN
1	T	59	SER
1	T	111	LEU
1	T	112	ASN

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Mol	Chain	Res	Type
1	T	114	ARG
2	B	15	SER
2	B	33[A]	ARG
2	B	33[B]	ARG
3	C	10	LEU
4	D	33[A]	LEU
4	D	33[B]	LEU
4	D	79	LYS
5	E	151	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	46	ASN
1	T	62	GLN
1	T	71	ASN
1	T	98	ASN
1	T	170	GLN
1	T	189	GLN
1	T	203	GLN
3	C	7	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)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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	$\#\|Z\| > 2$
7	GOL	T	4	-	5,5,5	0.77	0	5,5,5	1.95	2 (40%)
8	SO4	T	10	-	4,4,4	0.31	0	6,6,6	0.30	0
8	SO4	D	14	-	4,4,4	0.11	0	6,6,6	0.36	0
7	GOL	B	3	-	5,5,5	0.53	0	5,5,5	0.68	0
9	EDO	E	20	-	3,3,3	0.63	0	2,2,2	0.10	0
7	GOL	T	6	-	5,5,5	0.50	0	5,5,5	0.77	0
7	GOL	T	2	-	5,5,5	0.79	0	5,5,5	0.66	0
8	SO4	B	9	-	4,4,4	0.70	0	6,6,6	0.86	0
7	GOL	T	1	-	5,5,5	0.35	0	5,5,5	0.86	0
8	SO4	T	8	-	4,4,4	0.29	0	6,6,6	0.72	0
8	SO4	T	13	-	4,4,4	0.09	0	6,6,6	0.41	0
9	EDO	T	241	-	3,3,3	0.28	0	2,2,2	1.16	0
7	GOL	T	5	-	5,5,5	0.49	0	5,5,5	0.35	0
8	SO4	E	11	-	4,4,4	0.14	0	6,6,6	0.67	0
8	SO4	D	7	-	4,4,4	0.24	0	6,6,6	0.83	0
9	EDO	T	240	-	3,3,3	0.39	0	2,2,2	0.74	0
10	MRD	D	148	-	7,7,7	0.53	0	9,10,10	0.46	0
10	MRD	T	242	-	7,7,7	0.67	0	9,10,10	1.15	1 (11%)
9	EDO	T	239	-	3,3,3	0.27	0	2,2,2	1.09	0
9	EDO	D	147	-	3,3,3	0.49	0	2,2,2	0.66	0
9	EDO	E	21	-	3,3,3	0.39	0	2,2,2	1.25	0
8	SO4	E	15	-	4,4,4	0.07	0	6,6,6	0.37	0
8	SO4	B	12	-	4,4,4	0.47	0	6,6,6	0.44	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
7	GOL	T	2	-	-	1/4/4/4	-
10	MRD	D	148	-	-	0/5/5/5	-
7	GOL	T	4	-	-	4/4/4/4	-
7	GOL	T	5	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	T	239	-	-	0/1/1/1	-
9	EDO	D	147	-	-	1/1/1/1	-
7	GOL	T	1	-	-	2/4/4/4	-
9	EDO	E	21	-	-	1/1/1/1	-
9	EDO	T	240	-	-	0/1/1/1	-
7	GOL	B	3	-	-	2/4/4/4	-
9	EDO	T	241	-	-	0/1/1/1	-
9	EDO	E	20	-	-	1/1/1/1	-
7	GOL	T	6	-	-	0/4/4/4	-
10	MRD	T	242	-	-	2/5/5/5	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	4	GOL	O3-C3-C2	-3.35	94.14	110.20
10	T	242	MRD	O4-C4-C5	2.15	118.70	109.38
7	T	4	GOL	C3-C2-C1	-2.01	103.89	111.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	4	GOL	O1-C1-C2-C3
7	T	5	GOL	O1-C1-C2-C3
10	T	242	MRD	C1-C2-C3-C4
10	T	242	MRD	O2-C2-C3-C4
9	E	20	EDO	O1-C1-C2-O2
7	T	1	GOL	C1-C2-C3-O3
7	T	2	GOL	C1-C2-C3-O3
7	T	4	GOL	C1-C2-C3-O3
7	T	5	GOL	C1-C2-C3-O3
7	B	3	GOL	O1-C1-C2-C3
7	T	4	GOL	O1-C1-C2-O2
7	T	5	GOL	O1-C1-C2-O2
7	T	4	GOL	O2-C2-C3-O3
7	B	3	GOL	O1-C1-C2-O2
9	D	147	EDO	O1-C1-C2-O2
9	E	21	EDO	O1-C1-C2-O2
7	T	1	GOL	O2-C2-C3-O3
7	T	5	GOL	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	4	GOL	5	0
9	E	20	EDO	1	0
7	T	6	GOL	1	0
7	T	2	GOL	1	0
7	T	1	GOL	1	0
8	T	8	SO4	1	0
7	T	5	GOL	4	0
9	T	240	EDO	1	0
10	T	242	MRD	6	0
9	T	239	EDO	2	0
9	D	147	EDO	2	0
8	B	12	SO4	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	T	223/223 (100%)	-0.64	2 (0%) 84 87	11, 19, 30, 42	2 (0%)
2	B	61/61 (100%)	-0.36	4 (6%) 18 19	13, 18, 34, 54	5 (8%)
3	C	11/11 (100%)	-0.10	1 (9%) 9 9	19, 24, 34, 44	0
4	D	131/131 (100%)	-0.54	2 (1%) 73 77	12, 21, 34, 47	3 (2%)
5	E	96/96 (100%)	-0.52	3 (3%) 49 51	10, 17, 37, 47	2 (2%)
All	All	522/522 (100%)	-0.55	12 (2%) 60 64	10, 19, 34, 54	12 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	SER	8.0
4	D	76[A]	SER	3.4
3	C	11	SER	3.1
1	T	112	ASN	3.0
5	E	204	ASN	2.9
2	B	74	SER	2.7
5	E	151	THR	2.7
4	D	77	SER	2.5
1	T	142	SER	2.4
2	B	14	SER	2.3
2	B	17	PRO	2.2
5	E	150	ASN	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 (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^{th} 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
7	GOL	B	3	6/6	0.76	0.15	35,46,47,48	0
7	GOL	T	1	6/6	0.78	0.18	33,44,49,54	0
7	GOL	T	5	6/6	0.82	0.13	42,45,46,46	0
7	GOL	T	6	6/6	0.83	0.17	51,54,54,55	0
7	GOL	T	2	6/6	0.83	0.19	31,41,42,49	0
8	SO4	D	14	5/5	0.87	0.17	22,28,32,34	5
9	EDO	T	241	4/4	0.87	0.15	39,43,48,49	0
8	SO4	B	12	5/5	0.88	0.27	25,29,31,35	5
9	EDO	D	147	4/4	0.89	0.09	27,29,31,43	0
9	EDO	E	20	4/4	0.89	0.17	36,43,46,49	0
9	EDO	E	21	4/4	0.91	0.19	39,44,46,47	0
8	SO4	T	13	5/5	0.92	0.12	31,33,37,39	5
10	MRD	D	148	8/8	0.93	0.10	29,31,32,32	0
8	SO4	B	9	5/5	0.94	0.12	34,36,42,44	0
9	EDO	T	239	4/4	0.94	0.13	30,37,38,45	0
9	EDO	T	240	4/4	0.94	0.18	29,38,42,49	0
7	GOL	T	4	6/6	0.94	0.12	35,37,38,40	0
8	SO4	E	15	5/5	0.95	0.13	25,28,31,31	5
10	MRD	T	242	8/8	0.95	0.09	20,22,31,35	0
8	SO4	D	7	5/5	0.95	0.09	19,22,26,28	5
8	SO4	E	11	5/5	0.97	0.16	54,55,57,57	0
8	SO4	T	8	5/5	0.98	0.17	36,39,42,42	0
8	SO4	T	10	5/5	0.99	0.09	44,44,48,49	0
6	CA	T	300	1/1	1.00	0.03	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.