Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:53 AM GMT

PDB ID	:	2J3Z
Title	:	CRYSTAL STRUCTURE OF THE ENZYMATIC COMPONENT C2-I OF THE C2-TOXIN FROM CLOSTRIDIUM BOTULINUM AT PH 6.1
Authors	:	Schleberger, C.; Hochmann, H.; Barth, H.; Aktories, K.; Schulz, G.E.
Deposited on	:	2006-08-23
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

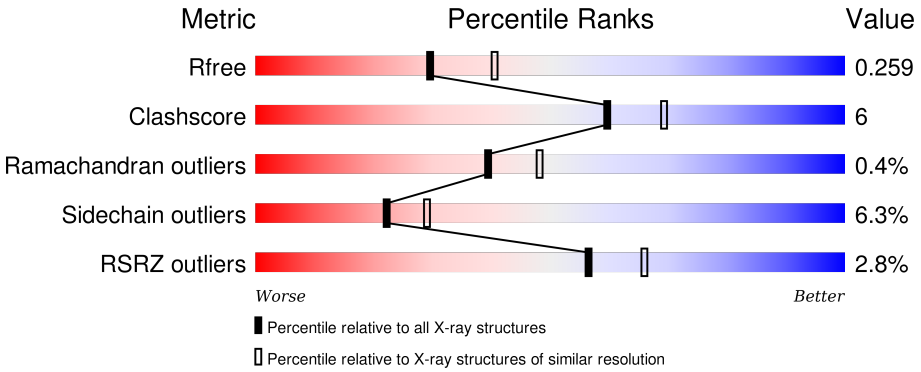
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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.



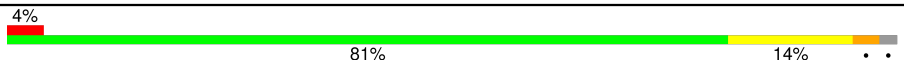
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	A	431	3% 80% 18%
1	B	431	2% 82% 16%
1	C	431	2% 85% 13%
1	D	431	2% 79% 16%
1	E	431	3% 82% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	431	

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
3	GOL	A	1433	-	-	-	X
3	GOL	A	1434	-	-	-	X
3	GOL	A	1435	-	-	-	X
3	GOL	A	1436	-	-	-	X
3	GOL	B	1434	-	-	-	X
3	GOL	B	1435	-	-	-	X
3	GOL	C	1431	-	-	-	X
3	GOL	C	1432	-	-	-	X
3	GOL	E	1430	-	-	-	X
3	GOL	F	1428	-	-	-	X
4	SO4	A	1437	-	-	-	X
4	SO4	B	1437	-	-	-	X
4	SO4	B	1439	-	-	-	X
4	SO4	B	1440	-	-	-	X
4	SO4	C	1439	-	-	-	X
4	SO4	D	1433	-	-	-	X
4	SO4	D	1434	-	-	-	X
4	SO4	E	1432	-	-	-	X
4	SO4	E	1433	-	-	-	X
4	SO4	F	1431	-	-	-	X
4	SO4	F	1433	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21502 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 C2 TOXIN COMPONENT I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3476	2216	575	683	2			
1	B	430	Total	C	N	O	S	0	0	0
			3476	2216	575	683	2			
1	C	428	Total	C	N	O	S	0	0	0
			3459	2205	573	679	2			
1	D	421	Total	C	N	O	S	0	0	0
			3401	2167	562	670	2			
1	E	423	Total	C	N	O	S	0	0	0
			3418	2176	566	674	2			
1	F	421	Total	C	N	O	S	0	0	0
			3401	2167	562	670	2			

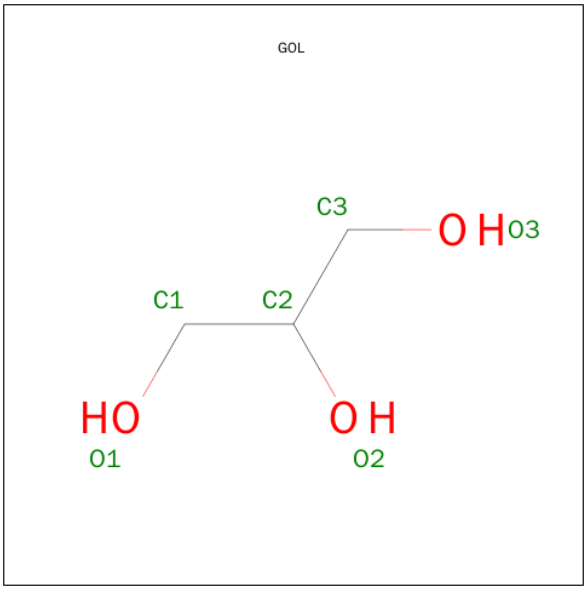
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ARG	HIS	ENGINEERED MUTATION	UNP O69275
B	77	ARG	HIS	ENGINEERED MUTATION	UNP O69275
C	77	ARG	HIS	ENGINEERED MUTATION	UNP O69275
D	77	ARG	HIS	ENGINEERED MUTATION	UNP O69275
E	77	ARG	HIS	ENGINEERED MUTATION	UNP O69275
F	77	ARG	HIS	ENGINEERED MUTATION	UNP O69275
A	121	ASP	ASN	CONFLICT	UNP O69275
B	121	ASP	ASN	CONFLICT	UNP O69275
C	121	ASP	ASN	CONFLICT	UNP O69275
D	121	ASP	ASN	CONFLICT	UNP O69275
E	121	ASP	ASN	CONFLICT	UNP O69275
F	121	ASP	ASN	CONFLICT	UNP O69275

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Co 1 1	0	0
2	E	1	Total Co 1 1	0	0
2	B	2	Total Co 2 2	0	0
2	C	1	Total Co 1 1	0	0
2	A	1	Total Co 1 1	0	0
2	F	1	Total Co 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



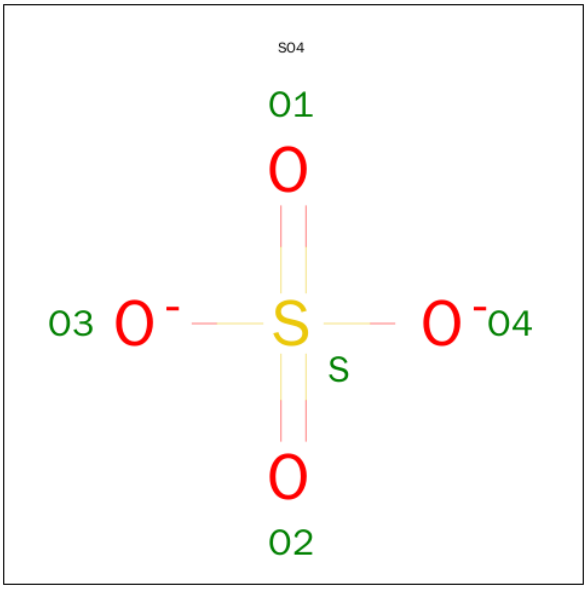
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	103	Total O 103 103	0	0
5	B	97	Total O 97 97	0	0
5	C	119	Total O 119 119	0	0
5	D	86	Total O 86 86	0	0
5	E	98	Total O 98 98	0	0

Continued on next page...

Continued from previous page...

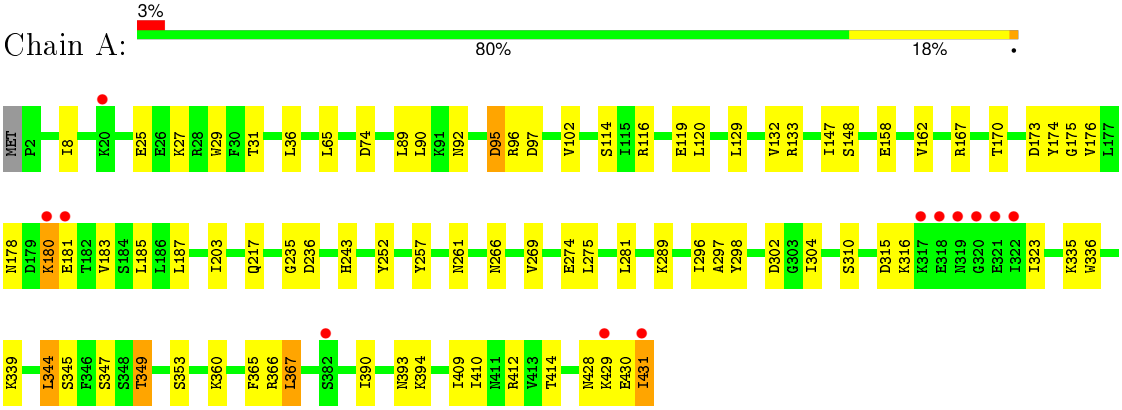
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	89	Total O 89 89	0	0

3 Residue-property plots (i)

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.

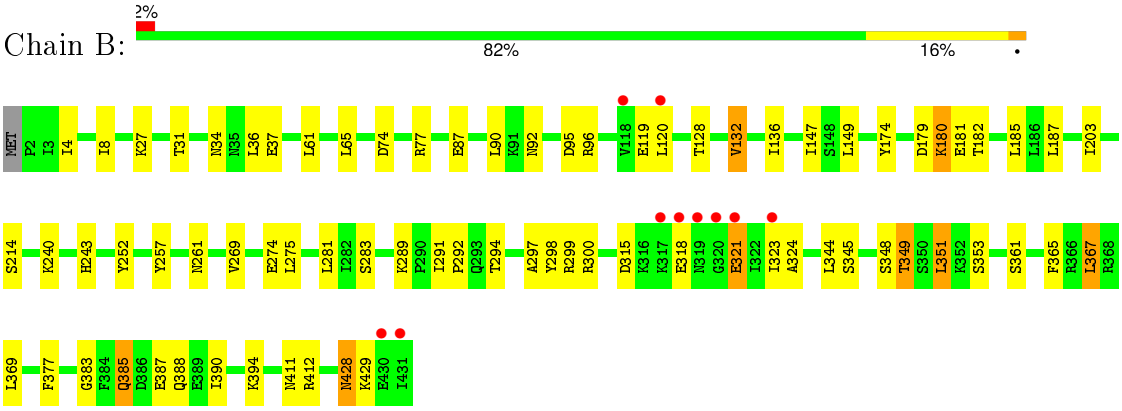
- Molecule 1: C2 TOXIN COMPONENT I

Chain A:



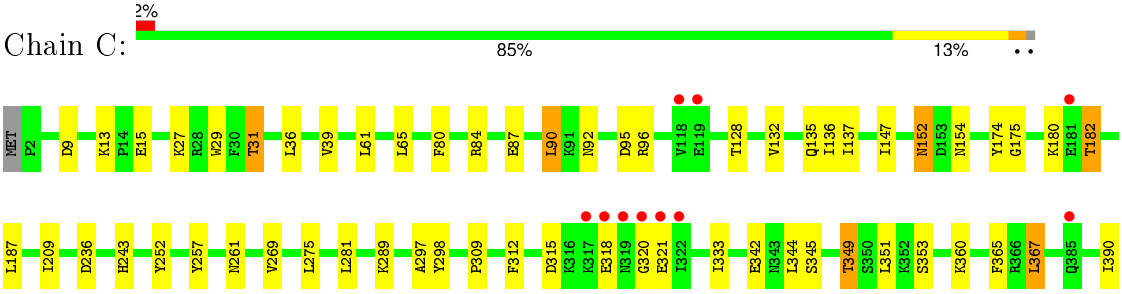
- Molecule 1: C2 TOXIN COMPONENT I

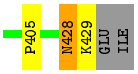
Chain B:



- Molecule 1: C2 TOXIN COMPONENT I

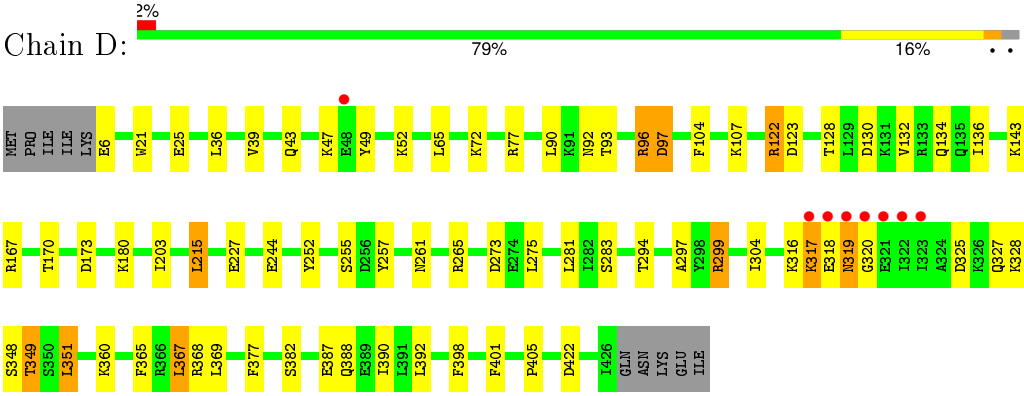
Chain C:





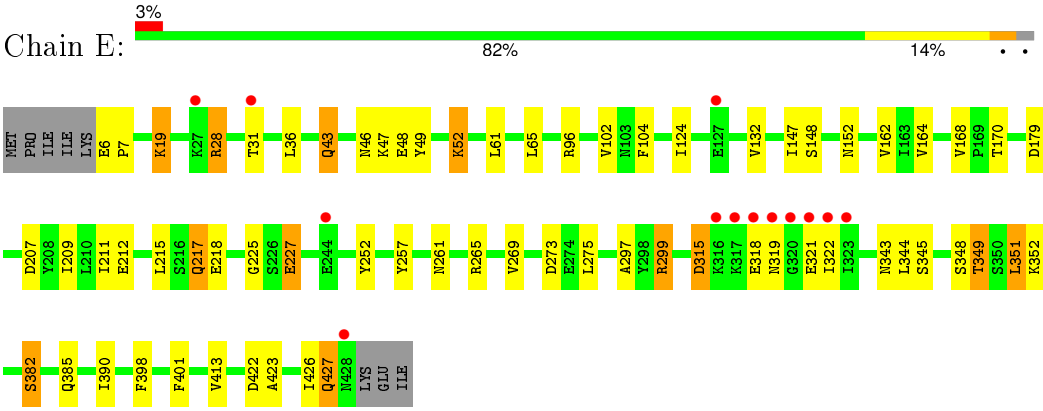
• Molecule 1: C2 TOXIN COMPONENT I

Chain D:



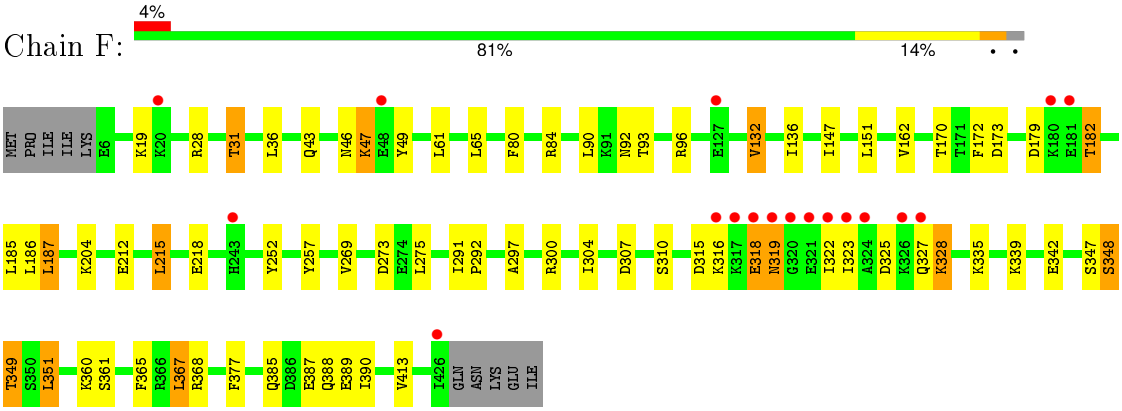
• Molecule 1: C2 TOXIN COMPONENT I

Chain E:



• Molecule 1: C2 TOXIN COMPONENT I

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	93.42Å 272.90Å 246.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 46.29 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.30) 92.7 (46.29-2.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	22.11 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.258 0.200 , 0.259	Depositor DCC
R_{free} test set	2650 reflections (2.04%)	DCC
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 137793 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21502	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CO, SO4

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	0.68	0/3537	0.75	0/4771
1	B	0.70	0/3537	0.77	0/4771
1	C	0.68	0/3520	0.78	1/4748 (0.0%)
1	D	0.75	2/3461 (0.1%)	0.79	5/4670 (0.1%)
1	E	0.66	0/3478	0.78	1/4693 (0.0%)
1	F	0.78	3/3461 (0.1%)	0.79	3/4670 (0.1%)
All	All	0.71	5/20994 (0.0%)	0.78	10/28323 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	328	LYS	CE-NZ	19.60	1.98	1.49
1	D	317	LYS	CE-NZ	14.63	1.85	1.49
1	D	317	LYS	CD-CE	8.74	1.73	1.51
1	F	327	GLN	CD-NE2	7.13	1.50	1.32
1	F	318	GLU	CD-OE1	5.21	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	317	LYS	CD-CE-NZ	-8.07	93.15	111.70
1	D	299	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	F	328	LYS	CD-CE-NZ	-6.03	97.83	111.70
1	D	368	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	95	ASP	CB-CA-C	-5.66	99.08	110.40
1	F	215	LEU	CA-CB-CG	5.45	127.84	115.30
1	F	368	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	D	215	LEU	CA-CB-CG	5.43	127.79	115.30
1	D	97	ASP	CB-CG-OD1	5.42	123.18	118.30
1	E	299	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	428	ASN	Peptide
1	B	428	ASN	Peptide

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	3476	0	3484	52	0
1	B	3476	0	3484	45	0
1	C	3459	0	3467	32	0
1	D	3401	0	3397	37	1
1	E	3418	0	3411	40	1
1	F	3401	0	3397	39	1
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	24	0	32	0	0
3	B	12	0	16	2	0
3	C	12	0	16	1	0
3	D	12	0	16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	6	0	8	2	0
3	F	6	0	8	0	0
4	A	25	0	0	0	0
4	B	40	0	0	1	0
4	C	35	0	0	0	0
4	D	30	0	0	0	0
4	E	35	0	0	0	0
4	F	35	0	0	0	0
5	A	103	0	0	3	0
5	B	97	0	0	1	0
5	C	119	0	0	2	0
5	D	86	0	0	1	0
5	E	98	0	0	4	0
5	F	89	0	0	0	0
All	All	21502	0	20736	236	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (236) 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:D:317:LYS:CE	1:D:317:LYS:NZ	1.85	1.39
1:F:328:LYS:NZ	1:F:328:LYS:CE	1.98	1.25
1:A:394:LYS:HZ3	1:A:431:ILE:HG21	1.22	1.02
1:E:299:ARG:HA	3:E:1430:GOL:H32	1.43	0.96
1:D:39:VAL:O	1:D:43:GLN:HG3	1.68	0.92
1:E:43:GLN:HB3	1:E:49:TYR:CE1	2.06	0.91
1:E:46:ASN:HD22	1:E:49:TYR:H	1.22	0.87
1:E:43:GLN:HB3	1:E:49:TYR:CD1	2.13	0.84
1:D:297:ALA:HB1	1:D:349:THR:HG23	1.61	0.83
1:A:235:GLY:HA3	1:E:382:SER:HB3	1.63	0.81
1:A:394:LYS:NZ	1:A:431:ILE:HG21	1.96	0.80
1:B:321:GLU:OE1	1:B:323:ILE:HB	1.83	0.79
1:C:365:PHE:HB3	1:C:367:LEU:HD13	1.65	0.78
1:A:25:GLU:HB2	1:A:176:VAL:HG21	1.67	0.76
1:B:323:ILE:HD12	1:B:324:ALA:H	1.52	0.75
1:F:179:ASP:HB3	1:F:182:THR:HG23	1.68	0.75
1:F:297:ALA:HB1	1:F:349:THR:HG23	1.69	0.75
1:A:25:GLU:CB	1:A:176:VAL:HG21	2.18	0.73
1:E:46:ASN:ND2	1:E:49:TYR:H	1.87	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ALA:HB1	1:E:349:THR:HG23	1.73	0.71
1:E:132:VAL:HG21	1:E:209:ILE:HD13	1.74	0.70
1:A:297:ALA:HB1	1:A:349:THR:HG23	1.75	0.69
1:E:52:LYS:HB3	1:E:52:LYS:HZ2	1.59	0.68
1:E:52:LYS:HB3	1:E:52:LYS:NZ	2.09	0.68
1:B:365:PHE:HB3	1:B:367:LEU:HD13	1.76	0.68
1:B:297:ALA:HB1	1:B:349:THR:HG23	1.76	0.66
1:B:387:GLU:HG2	3:B:1435:GOL:H32	1.77	0.66
1:A:116:ARG:NH2	1:A:158:GLU:O	2.28	0.66
1:A:147:ILE:CG2	1:A:187:LEU:HB2	2.26	0.65
1:B:92:ASN:HB3	1:B:174:TYR:O	1.96	0.65
1:E:349:THR:HG22	1:E:390:ILE:HB	1.77	0.65
1:D:317:LYS:CD	1:D:317:LYS:NZ	2.60	0.64
1:D:107:LYS:HB2	1:D:107:LYS:NZ	2.12	0.64
1:C:261:ASN:ND2	1:C:345:SER:HB2	2.13	0.63
1:A:92:ASN:HB3	1:A:174:TYR:O	1.98	0.63
1:D:261:ASN:OD1	1:D:345:SER:OG	2.17	0.63
1:F:47:LYS:HE3	1:F:47:LYS:H	1.62	0.63
1:F:413:VAL:O	1:F:413:VAL:HG22	2.00	0.62
1:A:335:LYS:O	1:A:339:LYS:HE3	1.99	0.62
1:B:269:VAL:CG2	1:D:360:LYS:HE3	2.29	0.62
1:A:269:VAL:HG23	1:F:360:LYS:HE3	1.81	0.62
1:E:261:ASN:OD1	1:E:345:SER:OG	2.17	0.62
1:C:92:ASN:HB3	1:C:174:TYR:O	1.99	0.61
1:C:297:ALA:HB1	1:C:349:THR:HG23	1.82	0.61
1:F:316:LYS:HE2	1:F:325:ASP:HA	1.83	0.61
1:A:393:ASN:HD21	1:A:431:ILE:CG2	2.13	0.60
1:E:318:GLU:O	1:E:319:ASN:CB	2.48	0.60
1:E:318:GLU:O	1:E:319:ASN:HB3	2.01	0.60
1:D:297:ALA:HB1	1:D:349:THR:CG2	2.31	0.60
1:D:52:LYS:HE2	1:D:77:ARG:HH12	1.66	0.60
1:A:147:ILE:HG22	1:A:187:LEU:HB2	1.84	0.59
1:B:128:THR:O	1:B:132:VAL:HG13	2.03	0.59
1:B:182:THR:HG22	5:B:2048:HOH:O	2.03	0.58
1:D:52:LYS:HE2	1:D:77:ARG:NH1	2.18	0.58
1:B:261:ASN:ND2	1:B:345:SER:HB2	2.19	0.58
1:D:349:THR:HG22	1:D:390:ILE:HB	1.86	0.58
1:B:383:GLY:H	1:B:385:GLN:HE21	1.52	0.58
1:A:8:ILE:HG13	1:A:96:ARG:HD2	1.85	0.57
1:D:43:GLN:HB2	1:D:49:TYR:CE1	2.40	0.57
1:D:365:PHE:HB3	1:D:367:LEU:HD13	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:ASP:OD2	1:E:322:ILE:HG22	2.05	0.56
1:A:236:ASP:OD1	1:A:289:LYS:NZ	2.37	0.56
1:B:269:VAL:HG23	1:D:360:LYS:HE3	1.86	0.56
1:B:365:PHE:HB3	1:B:367:LEU:CD1	2.35	0.56
1:A:97:ASP:OD2	1:A:167:ARG:NH1	2.34	0.56
1:E:261:ASN:O	1:E:265:ARG:HG3	2.06	0.56
1:D:329:LEU:HD22	1:D:405:PRO:HB3	1.88	0.56
1:F:365:PHE:HB3	1:F:367:LEU:HD13	1.87	0.55
1:F:335:LYS:O	1:F:339:LYS:HE3	2.07	0.55
1:F:93:THR:HG22	1:F:173:ASP:OD2	2.06	0.55
1:B:147:ILE:CG2	1:B:187:LEU:HB2	2.37	0.55
1:B:147:ILE:HG22	1:B:187:LEU:HB2	1.89	0.55
1:E:6:GLU:N	1:E:7:PRO:CD	2.71	0.54
1:A:316:LYS:HE3	1:A:323:ILE:HD11	1.90	0.54
1:A:349:THR:HG22	1:A:390:ILE:HB	1.90	0.54
1:B:8:ILE:HG13	1:B:96:ARG:HD2	1.90	0.54
1:F:151:LEU:HD21	1:F:185:LEU:HG	1.90	0.54
1:D:128:THR:O	1:D:132:VAL:HG13	2.08	0.54
1:F:297:ALA:HB1	1:F:349:THR:CG2	2.36	0.54
1:B:27:LYS:O	1:B:31:THR:HG23	2.07	0.54
1:F:328:LYS:CD	1:F:328:LYS:NZ	2.70	0.54
1:A:298:TYR:CG	1:A:353:SER:HA	2.43	0.54
1:C:128:THR:O	1:C:132:VAL:HG13	2.07	0.54
1:F:46:ASN:HB3	1:F:49:TYR:CD1	2.44	0.53
1:A:393:ASN:HD21	1:A:431:ILE:HG23	1.74	0.53
1:D:21:TRP:CZ2	1:D:25:GLU:HG3	2.44	0.53
1:C:252:TYR:O	1:C:257:TYR:HB3	2.09	0.52
1:C:27:LYS:O	1:C:31:THR:HG23	2.10	0.52
1:D:122:ARG:HD3	1:D:123:ASP:OD2	2.10	0.52
1:D:93:THR:HG22	1:D:173:ASP:OD2	2.09	0.52
1:B:351:LEU:HD22	1:B:377:PHE:HE2	1.75	0.52
1:E:28:ARG:O	1:E:31:THR:HG22	2.09	0.52
1:B:283:SER:OG	1:B:394:LYS:NZ	2.43	0.52
1:A:25:GLU:HB3	1:A:176:VAL:HG21	1.91	0.52
1:A:27:LYS:O	1:A:31:THR:HG23	2.09	0.52
1:B:349:THR:HG22	1:B:390:ILE:HB	1.92	0.51
1:F:28:ARG:O	1:F:31:THR:HG22	2.09	0.51
1:B:299:ARG:HA	3:B:1434:GOL:H11	1.92	0.51
1:C:132:VAL:HG21	1:C:209:ILE:HD13	1.93	0.51
1:B:297:ALA:HB1	1:B:349:THR:CG2	2.41	0.51
1:C:36:LEU:HA	1:C:39:VAL:HG12	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLU:HB2	1:D:96:ARG:HH21	1.76	0.50
1:A:243:HIS:HE1	1:B:243:HIS:CE1	2.28	0.50
1:A:360:LYS:HE3	1:F:269:VAL:CG2	2.42	0.50
1:F:19:LYS:NZ	1:F:179:ASP:O	2.45	0.50
1:C:349:THR:HG22	1:C:390:ILE:HB	1.92	0.50
1:D:294:THR:HA	1:D:369:LEU:O	2.12	0.50
1:F:349:THR:HG22	1:F:390:ILE:HB	1.93	0.49
1:A:243:HIS:CE1	1:B:243:HIS:CE1	2.99	0.49
1:A:261:ASN:OD1	1:A:345:SER:OG	2.23	0.49
1:A:89:LEU:O	1:A:173:ASP:HB3	2.12	0.49
1:F:318:GLU:HB3	1:F:323:ILE:HD11	1.94	0.49
1:C:15:GLU:HG2	1:C:154:ASN:OD1	2.13	0.49
1:C:182:THR:HG23	5:C:2054:HOH:O	2.13	0.49
1:C:90:LEU:HD13	5:C:2057:HOH:O	2.12	0.49
1:A:297:ALA:HB1	1:A:349:THR:CG2	2.43	0.48
1:D:97:ASP:OD2	1:D:167:ARG:HD3	2.13	0.48
1:C:236:ASP:OD1	1:C:289:LYS:NZ	2.47	0.48
1:F:318:GLU:O	1:F:319:ASN:HB3	2.14	0.48
1:B:180:LYS:O	1:B:181:GLU:HB2	2.14	0.48
1:A:410:ILE:HD12	1:A:414:THR:HG22	1.96	0.48
1:B:252:TYR:O	1:B:257:TYR:HB3	2.12	0.48
1:C:349:THR:HB	1:C:390:ILE:O	2.14	0.47
1:D:130:ASP:O	1:D:134:GLN:HG2	2.14	0.47
1:D:377:PHE:CZ	1:D:388:GLN:HA	2.48	0.47
1:B:34:ASN:OD1	1:B:37:GLU:HG3	2.14	0.47
1:C:365:PHE:HB3	1:C:367:LEU:CD1	2.41	0.47
1:F:46:ASN:HB3	1:F:49:TYR:HD1	1.80	0.47
1:D:104:PHE:CZ	1:D:143:LYS:HB2	2.50	0.47
1:A:336:TRP:HA	1:A:339:LYS:HG3	1.97	0.47
1:D:325:ASP:HB3	1:D:328:LYS:HB2	1.96	0.47
1:A:302:ASP:OD2	1:A:310:SER:HB2	2.15	0.47
1:A:296:ILE:HG21	1:A:366:ARG:HG3	1.97	0.47
1:C:147:ILE:HG23	1:C:187:LEU:HD12	1.97	0.47
3:E:1430:GOL:H31	5:E:2075:HOH:O	2.14	0.46
1:F:304:ILE:CD1	1:F:310:SER:HB3	2.44	0.46
1:E:147:ILE:CG2	1:E:187:LEU:HB2	2.45	0.46
1:C:428:ASN:O	1:C:429:LYS:HG3	2.16	0.46
1:E:227:GLU:H	1:E:227:GLU:HG2	1.61	0.46
1:A:365:PHE:HB3	1:A:367:LEU:HD13	1.98	0.46
1:B:240:LYS:HZ3	1:B:289:LYS:CE	2.28	0.46
1:C:9:ASP:H	3:C:1432:GOL:H31	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LEU:C	1:F:187:LEU:HG	2.31	0.46
1:E:343:ASN:ND2	5:E:2070:HOH:O	2.43	0.46
1:D:316:LYS:NZ	1:D:318:GLU:OE1	2.48	0.46
1:B:323:ILE:CD1	1:B:324:ALA:H	2.27	0.46
1:A:266:ASN:O	1:A:269:VAL:HG22	2.15	0.46
1:A:296:ILE:CG2	1:A:366:ARG:HG3	2.45	0.46
1:E:349:THR:CG2	1:E:390:ILE:HB	2.44	0.46
1:C:152:ASN:C	1:C:152:ASN:HD22	2.19	0.45
1:E:102:VAL:HA	1:E:148:SER:O	2.17	0.45
1:D:299:ARG:HH21	1:D:348:SER:HB3	1.81	0.45
1:F:147:ILE:CG2	1:F:187:LEU:HB2	2.47	0.45
1:E:19:LYS:NZ	1:E:179:ASP:O	2.49	0.45
1:A:176:VAL:HG12	1:A:185:LEU:HD22	1.99	0.45
1:C:27:LYS:O	1:C:31:THR:CG2	2.65	0.45
1:A:176:VAL:HG12	1:A:185:LEU:CD2	2.47	0.45
1:F:47:LYS:HE3	1:F:47:LYS:N	2.31	0.45
1:B:240:LYS:HZ3	1:B:289:LYS:HE2	1.82	0.45
1:A:252:TYR:O	1:A:257:TYR:HB3	2.17	0.45
1:E:401:PHE:CZ	1:E:422:ASP:HB3	2.52	0.44
1:D:6:GLU:HB2	1:D:96:ARG:NH2	2.32	0.44
1:C:298:TYR:CG	1:C:353:SER:HA	2.52	0.44
1:A:429:LYS:O	1:A:429:LYS:HG2	2.17	0.44
1:F:377:PHE:CZ	1:F:388:GLN:HA	2.53	0.44
1:A:412:ARG:CZ	5:A:2095:HOH:O	2.66	0.44
1:C:333:ILE:HD11	1:C:405:PRO:HG3	1.98	0.44
1:B:294:THR:HA	1:B:369:LEU:O	2.17	0.44
1:E:43:GLN:O	1:E:49:TYR:HD1	2.01	0.44
1:B:119:GLU:HG3	1:B:120:LEU:H	1.83	0.44
1:D:244:GLU:HG3	1:D:281:LEU:HD22	1.99	0.44
1:E:162:VAL:HG13	1:E:211:ILE:HD12	2.00	0.44
1:F:315:ASP:OD2	1:F:322:ILE:HG23	2.18	0.44
1:C:360:LYS:HE3	1:E:269:VAL:HG22	2.00	0.44
1:D:132:VAL:O	1:D:136:ILE:HG12	2.17	0.43
1:A:429:LYS:HB2	5:A:2100:HOH:O	2.19	0.43
1:E:351:LEU:HD22	1:E:377:PHE:HE2	1.83	0.43
1:D:401:PHE:CZ	1:D:422:ASP:HB3	2.53	0.43
1:F:304:ILE:HD11	1:F:310:SER:HB3	2.01	0.43
1:F:351:LEU:HD22	1:F:377:PHE:HE2	1.83	0.43
1:F:252:TYR:O	1:F:257:TYR:HB3	2.19	0.43
1:C:80:PHE:HB3	1:C:84:ARG:NH1	2.33	0.43
1:B:351:LEU:HD22	1:B:377:PHE:CE2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ASP:O	1:C:13:LYS:HD2	2.19	0.43
1:E:124:ILE:HG13	1:E:207:ASP:HB2	2.01	0.43
1:B:4:ILE:HB	1:F:172:PHE:CZ	2.54	0.43
1:F:47:LYS:CE	1:F:47:LYS:H	2.30	0.43
1:F:318:GLU:O	1:F:319:ASN:CB	2.67	0.43
1:A:304:ILE:HD11	1:A:310:SER:HB3	1.99	0.43
1:E:225:GLY:HA3	1:E:352:LYS:HG3	2.01	0.43
1:A:29:TRP:CZ3	1:A:175:GLY:HA3	2.54	0.42
1:B:351:LEU:HD12	1:B:351:LEU:HA	1.83	0.42
1:B:243:HIS:HE1	1:C:243:HIS:NE2	2.16	0.42
1:C:135:GLN:HB2	1:C:136:ILE:HG23	2.01	0.42
1:F:348:SER:HB2	1:F:389:GLU:OE2	2.19	0.42
1:B:300:ARG:HB3	1:B:361:SER:HB2	2.00	0.42
1:B:132:VAL:O	1:B:136:ILE:HG12	2.19	0.42
1:B:179:ASP:O	1:B:180:LYS:C	2.57	0.42
1:E:152:ASN:HB2	5:E:2001:HOH:O	2.19	0.42
1:E:398:PHE:HB3	1:E:423:ALA:HB1	2.02	0.42
1:A:430:GLU:O	1:A:431:ILE:HG22	2.20	0.41
1:B:349:THR:HB	1:B:390:ILE:O	2.20	0.41
1:F:132:VAL:O	1:F:136:ILE:HG12	2.19	0.41
1:B:298:TYR:CG	1:B:353:SER:HA	2.54	0.41
1:C:320:GLY:O	1:C:321:GLU:HG2	2.20	0.41
1:D:351:LEU:HD22	1:D:377:PHE:HE2	1.85	0.41
1:E:168:VAL:HG21	1:E:187:LEU:HD11	2.02	0.41
1:E:217:GLN:NE2	5:E:2045:HOH:O	2.43	0.41
1:A:102:VAL:HA	1:A:148:SER:O	2.20	0.41
1:B:149:LEU:HB3	1:B:185:LEU:HB2	2.02	0.41
1:D:387:GLU:HB3	5:D:2077:HOH:O	2.19	0.41
1:B:291:ILE:HA	1:B:292:PRO:HD3	1.98	0.41
1:A:29:TRP:CH2	1:A:175:GLY:HA3	2.56	0.41
1:E:426:ILE:HB	1:E:427:GLN:H	1.75	0.41
1:E:252:TYR:O	1:E:257:TYR:HB3	2.20	0.41
1:C:309:PRO:HD2	1:C:312:PHE:HB2	2.02	0.41
1:A:178:ASN:HD22	1:A:183:VAL:HG22	1.84	0.41
1:A:147:ILE:HG23	1:A:187:LEU:HB2	2.02	0.41
1:F:413:VAL:O	1:F:413:VAL:CG2	2.68	0.41
1:D:252:TYR:O	1:D:257:TYR:HB3	2.20	0.41
1:A:344:LEU:HD12	1:A:344:LEU:HA	1.88	0.41
1:D:392:LEU:HD13	1:D:398:PHE:HZ	1.86	0.41
1:F:300:ARG:HB3	1:F:361:SER:HB2	2.03	0.41
1:E:297:ALA:HB1	1:E:349:THR:CG2	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:PHE:CZ	1:B:388:GLN:HA	2.56	0.41
1:E:104:PHE:HB2	1:E:164:VAL:HG21	2.02	0.41
1:A:129:LEU:HD21	1:A:133:ARG:HH21	1.86	0.41
1:E:349:THR:HB	1:E:390:ILE:O	2.21	0.41
1:B:411:ASN:HB2	4:B:1437:SO4:O4	2.20	0.41
1:F:80:PHE:HB3	1:F:84:ARG:NH1	2.36	0.40
1:D:107:LYS:HB2	1:D:107:LYS:HZ2	1.86	0.40
1:C:137:ILE:HA	1:C:137:ILE:HD13	1.93	0.40
1:A:95:ASP:HB2	5:A:2046:HOH:O	2.21	0.40
1:F:291:ILE:HA	1:F:292:PRO:HD3	1.80	0.40
1:C:29:TRP:CH2	1:C:175:GLY:HA3	2.56	0.40
1:A:180:LYS:O	1:A:181:GLU:HG2	2.21	0.40

All (2) 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)
1:E:273:ASP:OD2	1:F:273:ASP:OD1[3_554]	1.71	0.49
1:D:273:ASP:OD1	1:D:273:ASP:OD2[3_554]	1.97	0.23

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	428/431 (99%)	410 (96%)	18 (4%)	0	100	100
1	B	428/431 (99%)	405 (95%)	20 (5%)	3 (1%)	26	31
1	C	426/431 (99%)	412 (97%)	13 (3%)	1 (0%)	52	64
1	D	419/431 (97%)	407 (97%)	9 (2%)	3 (1%)	26	31
1	E	421/431 (98%)	401 (95%)	19 (4%)	1 (0%)	52	64
1	F	419/431 (97%)	402 (96%)	15 (4%)	2 (0%)	34	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2541/2586 (98%)	2437 (96%)	94 (4%)	10 (0%)	39 48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	385	GLN
1	B	180	LYS
1	B	321	GLU
1	D	180	LYS
1	F	385	GLN
1	C	180	LYS
1	D	319	ASN
1	B	385	GLN
1	F	319	ASN
1	D	320	GLY

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	393/394 (100%)	369 (94%)	24 (6%)	23 30
1	B	393/394 (100%)	369 (94%)	24 (6%)	23 30
1	C	391/394 (99%)	372 (95%)	19 (5%)	31 41
1	D	384/394 (98%)	358 (93%)	26 (7%)	20 25
1	E	386/394 (98%)	358 (93%)	28 (7%)	17 22
1	F	384/394 (98%)	357 (93%)	27 (7%)	19 23
All	All	2331/2364 (99%)	2183 (94%)	148 (6%)	22 29

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	74	ASP
1	A	90	LEU
1	A	95	ASP
1	A	114	SER
1	A	119	GLU
1	A	120	LEU
1	A	132	VAL
1	A	162	VAL
1	A	170	THR
1	A	180	LYS
1	A	203	ILE
1	A	217	GLN
1	A	274	GLU
1	A	275	LEU
1	A	281	LEU
1	A	315	ASP
1	A	344	LEU
1	A	347	SER
1	A	349	THR
1	A	367	LEU
1	A	409	ILE
1	A	431	ILE
1	B	36	LEU
1	B	61	LEU
1	B	65	LEU
1	B	74	ASP
1	B	77	ARG
1	B	87	GLU
1	B	90	LEU
1	B	95	ASP
1	B	132	VAL
1	B	203	ILE
1	B	214	SER
1	B	274	GLU
1	B	275	LEU
1	B	281	LEU
1	B	315	ASP
1	B	318	GLU
1	B	344	LEU
1	B	348	SER
1	B	349	THR
1	B	351	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	367	LEU
1	B	412	ARG
1	B	428	ASN
1	B	429	LYS
1	C	31	THR
1	C	61	LEU
1	C	65	LEU
1	C	87	GLU
1	C	90	LEU
1	C	96	ARG
1	C	152	ASN
1	C	182	THR
1	C	269	VAL
1	C	275	LEU
1	C	281	LEU
1	C	315	ASP
1	C	318	GLU
1	C	342	GLU
1	C	344	LEU
1	C	349	THR
1	C	351	LEU
1	C	367	LEU
1	C	428	ASN
1	D	36	LEU
1	D	47	LYS
1	D	65	LEU
1	D	72	LYS
1	D	90	LEU
1	D	92	ASN
1	D	96	ARG
1	D	122	ARG
1	D	148	SER
1	D	162	VAL
1	D	170	THR
1	D	203	ILE
1	D	215	LEU
1	D	227	GLU
1	D	255	SER
1	D	265	ARG
1	D	275	LEU
1	D	283	SER
1	D	304	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	319	ASN
1	D	327	GLN
1	D	344	LEU
1	D	349	THR
1	D	351	LEU
1	D	367	LEU
1	D	382	SER
1	E	19	LYS
1	E	28	ARG
1	E	36	LEU
1	E	43	GLN
1	E	47	LYS
1	E	48	GLU
1	E	52	LYS
1	E	61	LEU
1	E	65	LEU
1	E	96	ARG
1	E	170	THR
1	E	203	ILE
1	E	212	GLU
1	E	215	LEU
1	E	217	GLN
1	E	218	GLU
1	E	227	GLU
1	E	275	LEU
1	E	315	ASP
1	E	321	GLU
1	E	344	LEU
1	E	348	SER
1	E	349	THR
1	E	351	LEU
1	E	367	LEU
1	E	382	SER
1	E	413	VAL
1	E	427	GLN
1	F	31	THR
1	F	36	LEU
1	F	43	GLN
1	F	47	LYS
1	F	61	LEU
1	F	65	LEU
1	F	90	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	92	ASN
1	F	96	ARG
1	F	132	VAL
1	F	162	VAL
1	F	170	THR
1	F	182	THR
1	F	187	LEU
1	F	204	LYS
1	F	212	GLU
1	F	215	LEU
1	F	218	GLU
1	F	275	LEU
1	F	307	ASP
1	F	342	GLU
1	F	347	SER
1	F	348	SER
1	F	349	THR
1	F	351	LEU
1	F	367	LEU
1	F	387	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	178	ASN
1	A	217	GLN
1	A	393	ASN
1	A	395	ASN
1	B	12	ASN
1	B	35	ASN
1	B	55	ASN
1	B	78	ASN
1	B	261	ASN
1	B	385	GLN
1	C	55	ASN
1	C	78	ASN
1	C	135	GLN
1	C	152	ASN
1	C	261	ASN
1	C	395	ASN
1	D	55	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	134	GLN
1	D	395	ASN
1	E	35	ASN
1	E	46	ASN
1	E	55	ASN
1	E	134	GLN
1	E	266	ASN
1	E	395	ASN
1	E	427	GLN
1	F	55	ASN
1	F	78	ASN
1	F	188	ASN

5.3.3 RNA

There are no RNA molecules 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

Of 59 ligands modelled in this entry, 7 are monoatomic - leaving 52 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	$\#\|Z\| > 2$
3	GOL	A	1433	-	5,5,5	0.47	0	5,5,5	0.32	0
3	GOL	A	1434	-	5,5,5	0.40	0	5,5,5	1.33	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	1435	-	5,5,5	0.30	0	5,5,5	0.67	0
3	GOL	A	1436	-	5,5,5	0.31	0	5,5,5	0.40	0
4	SO4	A	1437	-	4,4,4	0.37	0	6,6,6	0.58	0
4	SO4	A	1438	-	4,4,4	0.13	0	6,6,6	0.48	0
4	SO4	A	1439	-	4,4,4	0.08	0	6,6,6	0.16	0
4	SO4	A	1440	-	4,4,4	0.26	0	6,6,6	0.33	0
4	SO4	A	1441	-	4,4,4	0.11	0	6,6,6	0.10	0
3	GOL	B	1434	-	5,5,5	0.37	0	5,5,5	0.61	0
3	GOL	B	1435	-	5,5,5	0.59	0	5,5,5	0.86	0
4	SO4	B	1436	-	4,4,4	0.11	0	6,6,6	0.42	0
4	SO4	B	1437	-	4,4,4	0.22	0	6,6,6	0.45	0
4	SO4	B	1438	-	4,4,4	0.19	0	6,6,6	0.30	0
4	SO4	B	1439	-	4,4,4	0.16	0	6,6,6	0.41	0
4	SO4	B	1440	-	4,4,4	0.33	0	6,6,6	0.64	0
4	SO4	B	1441	-	4,4,4	0.30	0	6,6,6	0.38	0
4	SO4	B	1442	-	4,4,4	0.14	0	6,6,6	0.55	0
4	SO4	B	1443	-	4,4,4	0.24	0	6,6,6	0.22	0
3	GOL	C	1431	-	5,5,5	0.19	0	5,5,5	0.95	0
3	GOL	C	1432	-	5,5,5	0.25	0	5,5,5	0.55	0
4	SO4	C	1433	-	4,4,4	0.20	0	6,6,6	0.28	0
4	SO4	C	1434	-	4,4,4	0.12	0	6,6,6	0.20	0
4	SO4	C	1435	-	4,4,4	0.07	0	6,6,6	0.15	0
4	SO4	C	1436	-	4,4,4	0.21	0	6,6,6	0.20	0
4	SO4	C	1437	-	4,4,4	0.20	0	6,6,6	0.71	0
4	SO4	C	1438	-	4,4,4	0.24	0	6,6,6	0.15	0
4	SO4	C	1439	-	4,4,4	0.17	0	6,6,6	0.28	0
3	GOL	D	1428	-	5,5,5	0.36	0	5,5,5	0.52	0
3	GOL	D	1429	-	5,5,5	0.25	0	5,5,5	0.90	0
4	SO4	D	1430	-	4,4,4	0.09	0	6,6,6	0.44	0
4	SO4	D	1431	-	4,4,4	0.09	0	6,6,6	0.31	0
4	SO4	D	1432	-	4,4,4	0.06	0	6,6,6	0.25	0
4	SO4	D	1433	-	4,4,4	0.06	0	6,6,6	0.41	0
4	SO4	D	1434	-	4,4,4	0.15	0	6,6,6	0.22	0
4	SO4	D	1435	-	4,4,4	0.16	0	6,6,6	0.51	0
3	GOL	E	1430	-	5,5,5	0.29	0	5,5,5	0.61	0
4	SO4	E	1431	-	4,4,4	0.06	0	6,6,6	0.44	0
4	SO4	E	1432	-	4,4,4	0.34	0	6,6,6	0.47	0
4	SO4	E	1433	-	4,4,4	0.08	0	6,6,6	0.30	0
4	SO4	E	1434	-	4,4,4	0.07	0	6,6,6	0.38	0
4	SO4	E	1435	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	E	1436	-	4,4,4	0.11	0	6,6,6	0.20	0
4	SO4	E	1437	-	4,4,4	0.18	0	6,6,6	0.27	0
3	GOL	F	1428	-	5,5,5	0.27	0	5,5,5	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	F	1429	-	4,4,4	0.14	0	6,6,6	0.33	0
4	SO4	F	1430	-	4,4,4	0.08	0	6,6,6	0.19	0
4	SO4	F	1431	-	4,4,4	0.15	0	6,6,6	0.35	0
4	SO4	F	1432	-	4,4,4	0.28	0	6,6,6	0.46	0
4	SO4	F	1433	-	4,4,4	0.11	0	6,6,6	0.44	0
4	SO4	F	1434	-	4,4,4	0.16	0	6,6,6	0.32	0
4	SO4	F	1435	-	4,4,4	0.25	0	6,6,6	0.37	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
3	GOL	A	1433	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1434	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1435	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1436	-	-	0/4/4/4	0/0/0/0
4	SO4	A	1437	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1438	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1439	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1440	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1441	-	-	0/0/0/0	0/0/0/0
3	GOL	B	1434	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1435	-	-	0/4/4/4	0/0/0/0
4	SO4	B	1436	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1437	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1438	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1439	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1440	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1441	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1442	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1443	-	-	0/0/0/0	0/0/0/0
3	GOL	C	1431	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1432	-	-	0/4/4/4	0/0/0/0
4	SO4	C	1433	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1434	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1435	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1436	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1437	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1438	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1439	-	-	0/0/0/0	0/0/0/0
3	GOL	D	1428	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	1429	-	-	0/4/4/4	0/0/0/0
4	SO4	D	1430	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1431	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1432	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1433	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1434	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1435	-	-	0/0/0/0	0/0/0/0
3	GOL	E	1430	-	-	0/4/4/4	0/0/0/0
4	SO4	E	1431	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1432	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1433	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1434	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1435	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1436	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1437	-	-	0/0/0/0	0/0/0/0
3	GOL	F	1428	-	-	0/4/4/4	0/0/0/0
4	SO4	F	1429	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1430	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1431	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1432	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1433	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1434	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1435	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1434	GOL	O2-C2-C3	2.01	117.86	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1434	GOL	1	0
3	B	1435	GOL	1	0
4	B	1437	SO4	1	0
3	C	1432	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1430	GOL	2	0

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, 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	A	430/431 (99%)	0.01	12 (2%)	56	66	22, 33, 49, 78	1 (0%)
1	B	430/431 (99%)	0.01	10 (2%)	64	72	22, 34, 54, 81	1 (0%)
1	C	428/431 (99%)	-0.01	10 (2%)	64	72	22, 32, 48, 80	1 (0%)
1	D	421/431 (97%)	-0.06	8 (1%)	70	76	22, 35, 57, 89	1 (0%)
1	E	423/431 (98%)	0.04	13 (3%)	52	62	24, 35, 55, 73	1 (0%)
1	F	421/431 (97%)	0.13	18 (4%)	39	48	23, 37, 62, 117	1 (0%)
All	All	2553/2586 (98%)	0.02	71 (2%)	56	66	22, 34, 55, 117	6 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	12.0
1	B	320	GLY	6.9
1	F	319	ASN	6.9
1	B	319	ASN	6.7
1	F	317	LYS	6.6
1	C	319	ASN	6.5
1	B	321	GLU	6.3
1	A	319	ASN	5.7
1	F	322	ILE	5.2
1	F	320	GLY	5.0
1	B	318	GLU	5.0
1	A	431	ILE	4.4
1	D	320	GLY	4.4
1	B	430	GLU	4.4
1	D	319	ASN	4.3
1	C	318	GLU	4.2
1	E	320	GLY	4.1
1	C	320	GLY	3.8
1	E	319	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	323	ILE	3.7
1	F	426	ILE	3.6
1	C	317	LYS	3.6
1	A	181	GLU	3.5
1	F	127	GLU	3.5
1	F	318	GLU	3.5
1	D	317	LYS	3.5
1	E	321	GLU	3.5
1	E	428	ASN	3.4
1	A	429	LYS	3.3
1	A	318	GLU	3.2
1	F	327	GLN	3.2
1	E	322	ILE	3.2
1	C	321	GLU	3.2
1	A	321	GLU	3.2
1	F	48	GLU	3.2
1	B	317	LYS	3.1
1	E	127	GLU	3.1
1	F	180	LYS	3.1
1	C	385	GLN	3.1
1	A	320	GLY	3.0
1	F	326	LYS	3.0
1	D	321	GLU	3.0
1	C	181	GLU	2.9
1	A	180	LYS	2.8
1	A	317	LYS	2.7
1	D	318	GLU	2.6
1	E	317	LYS	2.6
1	D	322	ILE	2.6
1	F	181	GLU	2.6
1	E	318	GLU	2.5
1	F	321	GLU	2.5
1	F	323	ILE	2.5
1	F	316	LYS	2.5
1	E	31	THR	2.4
1	A	20	LYS	2.4
1	B	323	ILE	2.4
1	A	382	SER	2.3
1	F	324	ALA	2.3
1	B	118	VAL	2.3
1	D	323	ILE	2.3
1	F	20	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	2.3
1	C	119	GLU	2.2
1	E	27	LYS	2.2
1	F	243	HIS	2.2
1	E	244	GLU	2.1
1	C	118	VAL	2.1
1	E	316	LYS	2.0
1	A	322	ILE	2.0
1	C	322	ILE	2.0
1	D	48	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	E	1433	5/5	0.93	0.41	17.15	75,75,76,76	0
3	GOL	B	1435	6/6	0.66	0.32	10.29	45,52,55,56	0
4	SO4	B	1440	5/5	0.77	0.23	7.84	70,71,72,73	0
4	SO4	B	1437	5/5	0.87	0.23	6.78	64,65,66,68	0
4	SO4	D	1433	5/5	0.94	0.20	6.45	74,76,76,76	0
3	GOL	A	1433	6/6	0.82	0.20	6.20	49,52,53,53	0
4	SO4	F	1433	5/5	0.86	0.20	4.67	81,81,81,82	0
4	SO4	D	1434	5/5	0.82	0.24	4.06	92,92,93,93	0
3	GOL	B	1434	6/6	0.84	0.21	4.05	38,41,43,44	0
4	SO4	B	1439	5/5	0.88	0.20	4.02	71,71,71,72	0
3	GOL	E	1430	6/6	0.84	0.20	3.54	48,56,57,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	A	1434	6/6	0.88	0.19	3.51	39,40,43,43	0
3	GOL	F	1428	6/6	0.84	0.19	3.06	38,42,43,44	0
3	GOL	A	1435	6/6	0.80	0.23	3.05	60,61,61,62	0
4	SO4	E	1432	5/5	0.72	0.20	2.86	75,75,77,77	0
4	SO4	F	1431	5/5	0.92	0.18	2.55	64,66,67,67	0
3	GOL	C	1431	6/6	0.90	0.19	2.41	39,39,40,42	0
4	SO4	A	1437	5/5	0.88	0.16	2.38	59,60,62,63	0
3	GOL	C	1432	6/6	0.84	0.15	2.27	56,57,58,59	0
4	SO4	C	1439	5/5	0.91	0.15	2.27	72,72,73,74	0
3	GOL	A	1436	6/6	0.92	0.20	2.19	56,58,58,58	0
4	SO4	C	1434	5/5	0.95	0.15	1.85	73,73,73,74	0
3	GOL	D	1428	6/6	0.81	0.15	1.59	48,54,55,55	0
4	SO4	E	1435	5/5	0.90	0.14	0.86	62,64,64,65	0
4	SO4	F	1435	5/5	0.88	0.15	0.86	63,63,63,63	0
4	SO4	D	1435	5/5	0.92	0.14	0.82	64,64,66,66	0
3	GOL	D	1429	6/6	0.90	0.16	0.67	37,43,44,45	0
4	SO4	A	1439	5/5	0.95	0.14	0.43	70,71,71,71	0
4	SO4	A	1440	5/5	0.89	0.15	0.41	59,59,62,62	0
4	SO4	F	1429	5/5	0.85	0.14	0.18	77,79,80,80	0
4	SO4	C	1433	5/5	0.85	0.15	-0.17	70,71,72,73	0
4	SO4	B	1436	5/5	0.91	0.14	-0.52	71,72,73,73	0
4	SO4	F	1432	5/5	0.92	0.12	-0.77	64,66,66,66	0
4	SO4	B	1441	5/5	0.95	0.13	-1.00	55,55,56,57	0
4	SO4	A	1438	5/5	0.95	0.10	-1.01	75,75,76,76	0
4	SO4	C	1437	5/5	0.96	0.09	-1.26	52,55,56,56	0
2	CO	C	1430	1/1	0.97	0.13	-	51,51,51,51	0
4	SO4	C	1438	5/5	0.96	0.11	-	60,60,60,61	0
2	CO	A	1432	1/1	0.95	0.10	-	69,69,69,69	0
4	SO4	E	1434	5/5	0.90	0.20	-	79,79,80,80	0
4	SO4	A	1441	5/5	0.90	0.20	-	82,82,83,83	0
4	SO4	C	1436	5/5	0.85	0.22	-	78,79,79,80	0
4	SO4	D	1430	5/5	0.87	0.21	-	77,77,78,79	0
2	CO	E	1429	1/1	0.96	0.09	-	57,57,57,57	0
4	SO4	D	1431	5/5	0.91	0.37	-	75,75,75,76	0
4	SO4	D	1432	5/5	0.89	0.24	-	78,78,79,80	0
4	SO4	B	1442	5/5	0.82	0.18	-	76,77,78,78	0
2	CO	F	1427	1/1	0.99	0.10	-	55,55,55,55	0
2	CO	B	1432	1/1	0.99	0.09	-	46,46,46,46	0
2	CO	B	1433	1/1	0.96	0.14	-	64,64,64,64	0
4	SO4	C	1435	5/5	0.92	0.18	-	79,79,79,80	0
4	SO4	E	1437	5/5	0.89	0.32	-	74,75,75,76	0
4	SO4	E	1431	5/5	0.83	0.28	-	84,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	B	1443	5/5	0.87	0.15	-	73,74,75,75	0
4	SO4	F	1434	5/5	0.95	0.13	-	69,69,70,71	0
2	CO	D	1427	1/1	0.98	0.12	-	56,56,56,56	0
4	SO4	B	1438	5/5	0.90	0.13	-	68,69,70,70	0
4	SO4	F	1430	5/5	0.41	0.46	-	110,110,111,111	0
4	SO4	E	1436	5/5	0.96	0.10	-	62,63,63,64	0

6.5 Other polymers

There are no such residues in this entry.