



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:44 PM UTC

PDB ID : 1YQ2 / pdb_00001yq2
Title : beta-galactosidase from *Arthrobacter* sp. C2-2 (isoenzyme C2-2-1)
Authors : Skalova, T.; Dohnalek, J.; Spiwok, V.; Lipovova, P.; Vondrackova, E.;
Petrokova, H.; Strnad, H.; Kralova, B.; Hasek, J.
Deposited on : 2005-02-01
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

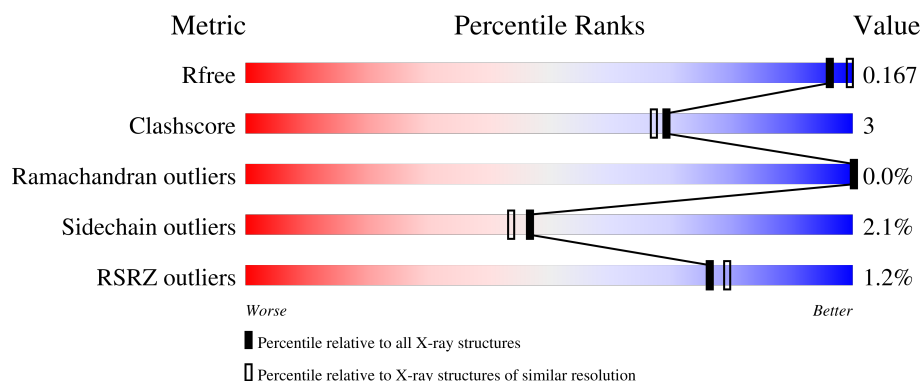
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	1024	91% 8%
1	B	1024	93% 6%
1	C	1024	94% 5%
1	D	1024	91% 8%
1	E	1024	92% 7%

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Mol	Chain	Length	Quality of chain
1	F	1024	% 91% 8% .

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
6	PEG	B	9002	-	-	X	-
6	PEG	C	9003	-	-	X	-
6	PEG	E	9005	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53897 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 beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1020	Total	C	N	O	S	0	17	0
			7882	4949	1419	1493	21			
1	B	1020	Total	C	N	O	S	0	15	0
			7870	4943	1422	1484	21			
1	C	1020	Total	C	N	O	S	0	19	0
			7891	4955	1426	1488	22			
1	D	1020	Total	C	N	O	S	0	14	0
			7870	4942	1416	1491	21			
1	E	1020	Total	C	N	O	S	0	17	0
			7888	4954	1426	1485	23			
1	F	1020	Total	C	N	O	S	0	20	0
			7904	4961	1436	1486	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q8KRF6
A	903	MET	VAL	engineered mutation	UNP Q8KRF6
B	0	HIS	-	expression tag	UNP Q8KRF6
B	903	MET	VAL	engineered mutation	UNP Q8KRF6
C	0	HIS	-	expression tag	UNP Q8KRF6
C	903	MET	VAL	engineered mutation	UNP Q8KRF6
D	0	HIS	-	expression tag	UNP Q8KRF6
D	903	MET	VAL	engineered mutation	UNP Q8KRF6
E	0	HIS	-	expression tag	UNP Q8KRF6
E	903	MET	VAL	engineered mutation	UNP Q8KRF6
F	0	HIS	-	expression tag	UNP Q8KRF6
F	903	MET	VAL	engineered mutation	UNP Q8KRF6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

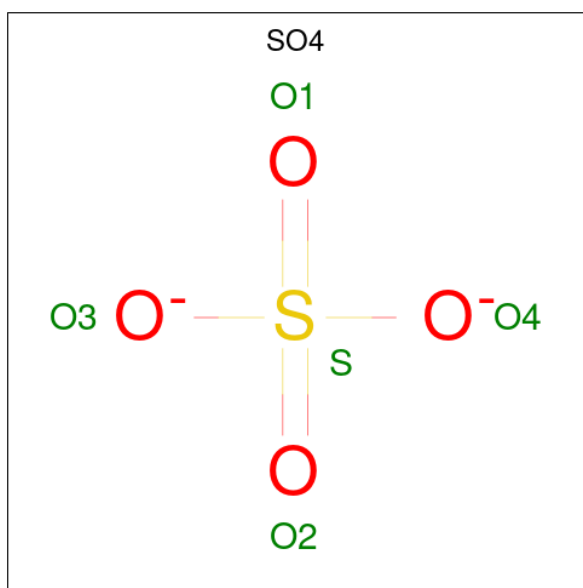
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0
3	B	2	Total Na 2 2	0	0
3	C	2	Total Na 2 2	0	0
3	D	2	Total Na 2 2	0	0
3	E	2	Total Na 2 2	0	0
3	F	2	Total Na 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

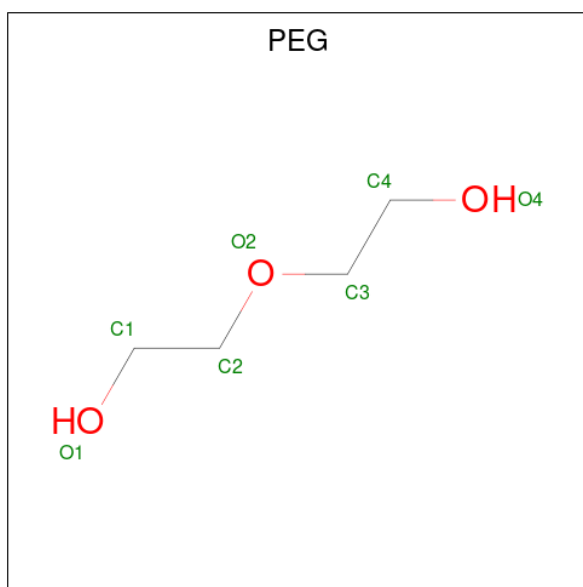
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

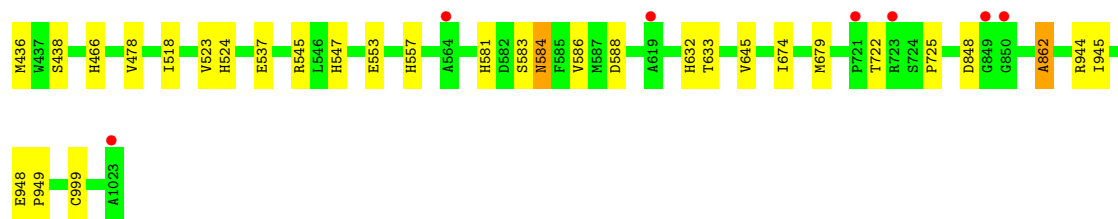
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



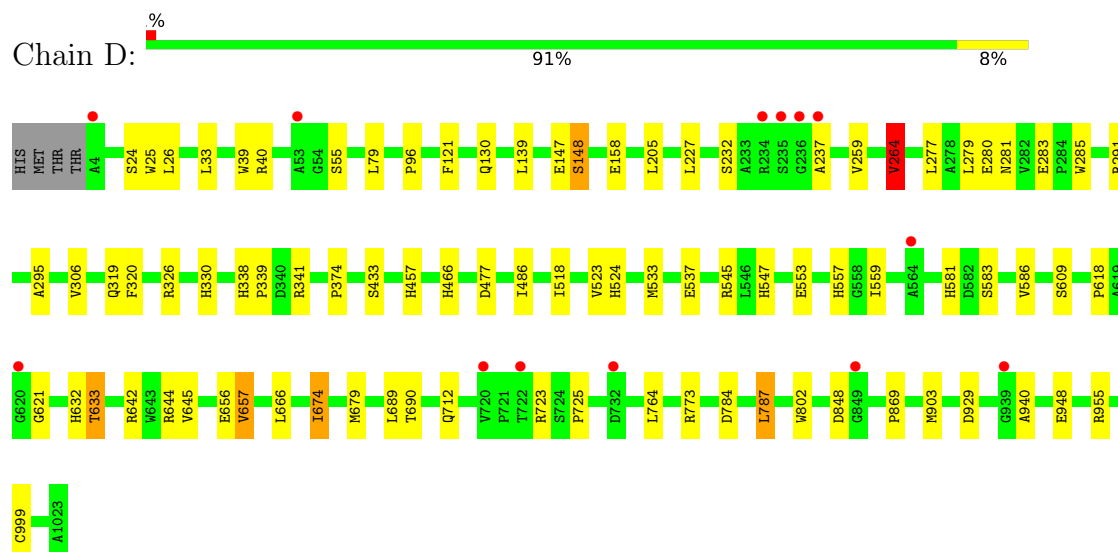
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		
6	E	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

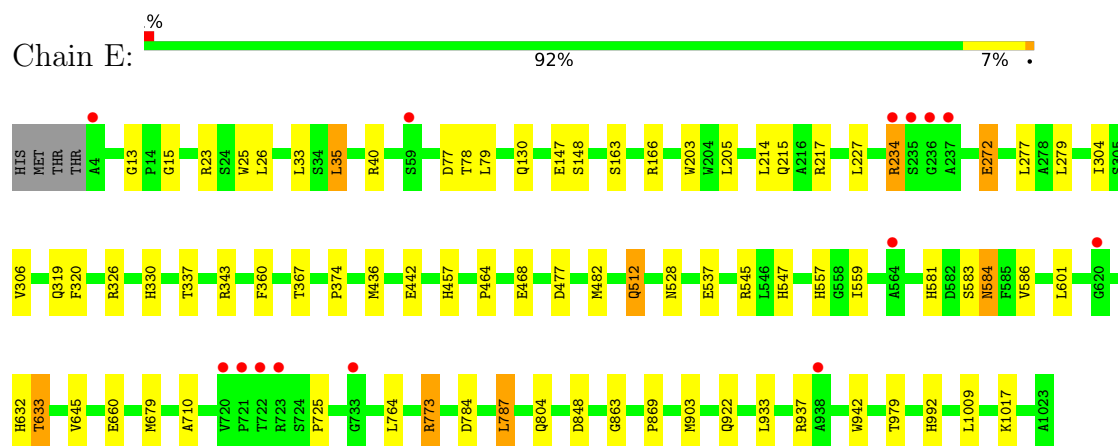
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1119	Total	O	0	0
			1119	1119		
7	B	1122	Total	O	0	0
			1122	1122		
7	C	1108	Total	O	0	0
			1108	1108		
7	D	1089	Total	O	0	0
			1089	1089		
7	E	969	Total	O	0	0
			969	969		
7	F	1064	Total	O	0	0
			1064	1064		



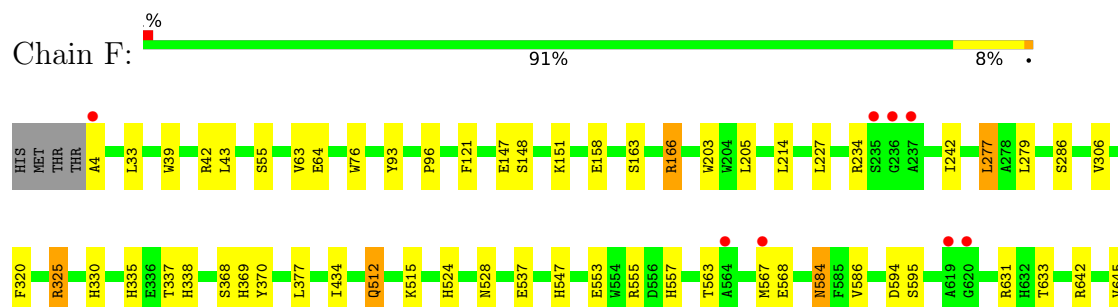
• Molecule 1: beta-galactosidase

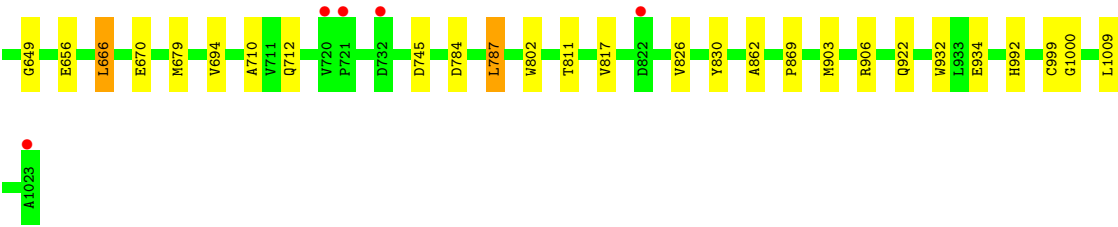


• Molecule 1: beta-galactosidase



• Molecule 1: beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	140.09Å 205.70Å 140.46Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.00-1.90) 95.0 (40.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.157 , 0.195 0.157 , 0.167	Depositor DCC
R_{free} test set	5792 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53897	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: SO4, PEG, MG, NA, CL

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	0.78	0/8190	0.86	3/11200 (0.0%)
1	B	0.80	1/8173 (0.0%)	0.87	9/11176 (0.1%)
1	C	0.78	0/8210	0.87	6/11226 (0.1%)
1	D	0.80	1/8157 (0.0%)	0.87	7/11157 (0.1%)
1	E	0.79	1/8198 (0.0%)	0.86	4/11207 (0.0%)
1	F	0.79	0/8226	0.87	4/11245 (0.0%)
All	All	0.79	3/49154 (0.0%)	0.87	33/67211 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	486	ILE	CA-CB	6.31	1.57	1.54
1	B	793	VAL	CA-CB	5.69	1.58	1.54
1	E	367	THR	CA-CB	5.59	1.60	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	862[A]	ALA	N-CA-C	-10.72	96.70	110.53
1	F	862[B]	ALA	N-CA-C	-10.72	96.70	110.53
1	C	862[A]	ALA	N-CA-C	-10.65	96.79	110.53
1	C	862[B]	ALA	N-CA-C	-10.65	96.79	110.53
1	D	609	SER	CA-C-N	7.52	127.16	119.56
1	D	609	SER	C-N-CA	7.52	127.16	119.56
1	A	15	GLY	N-CA-C	-6.37	105.10	111.85
1	E	863	GLY	N-CA-C	6.33	121.63	114.67
1	E	15	GLY	N-CA-C	-6.33	104.35	111.63
1	E	13	GLY	CA-C-N	6.32	126.44	119.87
1	E	13	GLY	C-N-CA	6.32	126.44	119.87
1	B	862	ALA	N-CA-C	6.12	118.92	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235[A]	SER	N-CA-C	5.98	123.53	110.80
1	B	235[B]	SER	N-CA-C	5.98	123.53	110.80
1	B	299	SER	N-CA-C	-5.72	101.45	109.69
1	C	13	GLY	CA-C-N	5.59	125.69	119.87
1	C	13	GLY	C-N-CA	5.59	125.69	119.87
1	F	1000	GLY	CA-C-N	5.57	125.52	119.78
1	F	1000	GLY	C-N-CA	5.57	125.52	119.78
1	B	148[A]	SER	CB-CA-C	-5.43	99.78	110.10
1	B	148[B]	SER	CB-CA-C	-5.43	99.78	110.10
1	D	264	VAL	N-CA-CB	5.43	116.64	110.72
1	A	123	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	A	862	ALA	N-CA-C	5.34	118.01	111.82
1	B	511	ARG	N-CA-CB	-5.28	102.35	110.01
1	D	940	ALA	CA-C-N	5.25	125.55	119.93
1	D	940	ALA	C-N-CA	5.25	125.55	119.93
1	D	148[A]	SER	CB-CA-C	-5.16	100.30	110.10
1	D	148[B]	SER	CB-CA-C	-5.16	100.30	110.10
1	B	793	VAL	CB-CA-C	5.09	115.07	110.13
1	B	277	LEU	CA-CB-CG	5.08	134.08	116.30
1	C	148[A]	SER	CB-CA-C	-5.04	100.52	110.10
1	C	148[B]	SER	CB-CA-C	-5.04	100.52	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7882	0	7501	62	0
1	B	7870	0	7495	48	0
1	C	7891	0	7512	42	0
1	D	7870	0	7479	57	0
1	E	7888	0	7517	56	0
1	F	7904	0	7537	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	10	0	0	0	0
6	A	7	0	10	3	0
6	B	7	0	10	4	0
6	C	7	0	10	4	0
6	D	7	0	10	3	0
6	E	7	0	10	6	0
6	F	7	0	10	3	0
7	A	1119	0	0	2	1
7	B	1122	0	0	9	0
7	C	1108	0	0	4	0
7	D	1089	0	0	7	0
7	E	969	0	0	4	0
7	F	1064	0	0	5	1
All	All	53897	0	45101	323	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 3.

All (323) 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:773:ARG:NH2	7:D:9615:HOH:O	1.95	0.99
1:C:227:LEU:HD12	1:C:306[A]:VAL:HG21	1.47	0.96
1:B:773:ARG:NH1	7:B:9651:HOH:O	1.97	0.96
1:F:227:LEU:HD12	1:F:306[A]:VAL:HG21	1.46	0.95
1:D:690:THR:HG23	1:D:903[B]:MET:CE	1.97	0.93
1:B:227:LEU:HD12	1:B:306[A]:VAL:HG21	1.48	0.93
1:C:227:LEU:HD12	1:C:306[B]:VAL:HG11	1.49	0.93
1:D:903[B]:MET:SD	7:D:9245:HOH:O	2.31	0.88
1:B:178:ARG:H	1:B:182:ASN:HD21	1.22	0.87
1:A:229:THR:HG21	1:A:309:GLY:O	1.73	0.86
1:B:632:HIS:ND1	1:B:633:THR:HG22	1.90	0.86
1:C:632:HIS:ND1	1:C:633:THR:HG23	1.92	0.84
1:A:237:ALA:HB1	1:A:283[B]:GLU:OE2	1.77	0.84
1:B:512:GLN:HE21	1:B:512:GLN:HA	1.43	0.82
1:F:512:GLN:HA	1:F:512:GLN:HE21	1.45	0.81
1:C:320:PHE:H	1:C:547:HIS:CE1	1.99	0.80
1:E:512:GLN:HE21	1:E:512:GLN:HA	1.47	0.80
1:D:227:LEU:HD12	1:D:306[A]:VAL:HG21	1.63	0.79
1:F:710:ALA:HB1	1:F:903[B]:MET:HE1	1.65	0.79
1:A:512:GLN:HE21	1:A:512:GLN:HA	1.47	0.79
1:D:320:PHE:H	1:D:547:HIS:CE1	2.02	0.78
1:A:280:GLU:CD	1:A:280:GLU:H	1.88	0.78
1:C:581:HIS:HD2	1:C:583:SER:H	1.27	0.78
1:E:992:HIS:HD2	1:E:1009:LEU:H	1.33	0.77
1:E:227:LEU:HD12	1:E:306:VAL:HG21	1.64	0.77
1:B:584:ASN:HD22	1:B:584:ASN:H	1.34	0.76
1:F:992:HIS:HD2	1:F:1009:LEU:H	1.33	0.76
1:D:690:THR:HG23	1:D:903[B]:MET:HE1	1.68	0.75
1:A:320:PHE:H	1:A:547:HIS:CE1	2.05	0.75
1:E:937:ARG:HG2	1:E:942:TRP:HB2	1.69	0.74
1:F:512:GLN:HE22	1:F:515[B]:LYS:NZ	1.85	0.74
1:F:320:PHE:H	1:F:547:HIS:CE1	2.07	0.72
1:F:335:HIS:HD2	7:F:9706:HOH:O	1.71	0.72
1:B:259:VAL:HB	1:B:264:VAL:HG13	1.72	0.71
1:F:227:LEU:CD1	1:F:306[A]:VAL:HG21	2.21	0.71
1:A:657:VAL:HG11	1:A:674:ILE:HD13	1.72	0.70
1:A:227:LEU:HD12	1:A:306:VAL:HG21	1.73	0.69
1:B:155:ASN:HD21	1:B:182:ASN:HD22	1.38	0.69
1:A:632:HIS:ND1	1:A:633:THR:HG22	2.06	0.69
1:D:581:HIS:HD2	1:D:583:SER:H	1.40	0.69
1:E:234:ARG:HG3	7:E:9792:HOH:O	1.93	0.69
1:B:784:ASP:HB3	1:B:787:LEU:HD22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:THR:CG2	1:D:903[B]:MET:CE	2.71	0.68
1:E:584:ASN:HD22	1:E:584:ASN:H	1.42	0.68
1:E:23:ARG:HH22	1:E:215:GLN:HE22	1.42	0.68
1:E:436[B]:MET:HG3	1:E:464:PRO:O	1.94	0.68
1:A:712:GLN:HG3	1:A:903[A]:MET:SD	2.34	0.68
1:E:320:PHE:H	1:E:547:HIS:CE1	2.12	0.67
1:A:657:VAL:HG11	1:A:674:ILE:CD1	2.25	0.66
1:A:710:ALA:HB1	1:A:903[A]:MET:HE1	1.77	0.66
1:E:581:HIS:HD2	1:E:583:SER:H	1.43	0.65
1:C:343:ARG:HH21	6:C:9003:PEG:H42	1.61	0.65
1:C:632:HIS:ND1	1:C:633:THR:CG2	2.60	0.65
1:B:283:GLU:HG2	7:B:9895:HOH:O	1.96	0.64
1:E:557:HIS:HB3	6:E:9005:PEG:H12	1.80	0.64
1:F:325[B]:ARG:HD3	7:F:9969:HOH:O	1.96	0.64
1:A:229:THR:HG23	1:A:310:PHE:HA	1.80	0.63
1:E:337:THR:OG1	1:E:557:HIS:HD2	1.80	0.63
1:B:557:HIS:HB2	1:B:586:VAL:HG22	1.81	0.63
1:F:557:HIS:HB3	6:F:9006:PEG:H12	1.80	0.63
1:C:335:HIS:NE2	6:C:9003:PEG:H41	2.12	0.63
1:E:319:GLN:HE22	1:E:326:ARG:HD2	1.63	0.62
1:E:457:HIS:HE1	1:E:477:ASP:OD2	1.82	0.62
1:F:992:HIS:CD2	1:F:1009:LEU:H	2.16	0.62
1:E:632:HIS:ND1	1:E:633:THR:HG22	2.14	0.62
1:F:512:GLN:HE22	1:F:515[B]:LYS:HZ3	1.46	0.62
1:A:229:THR:CG2	1:A:310:PHE:HA	2.29	0.62
1:D:633:THR:HG21	7:D:9036:HOH:O	1.99	0.62
1:C:584:ASN:H	1:C:584:ASN:HD22	1.47	0.62
1:E:343:ARG:HH11	6:E:9005:PEG:H42	1.65	0.62
1:A:457:HIS:HE1	1:A:477:ASP:OD2	1.83	0.61
1:C:645:VAL:HG21	1:C:679:MET:SD	2.41	0.61
1:F:33:LEU:HD11	1:F:214:LEU:HD12	1.83	0.60
1:E:337:THR:CB	1:E:557:HIS:HD2	2.15	0.60
1:A:33:LEU:HD12	1:A:35:LEU:HD13	1.82	0.60
1:D:319:GLN:HE22	1:D:326:ARG:HD2	1.66	0.60
1:A:151:LYS:HE3	1:A:158:GLU:CD	2.27	0.60
1:C:320:PHE:H	1:C:547:HIS:HE1	1.50	0.60
1:C:343:ARG:NH2	6:C:9003:PEG:H42	2.15	0.60
1:D:330:HIS:HE1	1:D:537:GLU:OE1	1.85	0.60
1:B:320:PHE:H	1:B:547:HIS:CE1	2.18	0.59
1:A:584:ASN:H	1:A:584:ASN:HD22	1.51	0.59
1:A:642:ARG:HG2	1:A:656:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:THR:HG23	1:D:903[B]:MET:HE2	1.84	0.59
1:F:642:ARG:HG2	1:F:656:GLU:HG2	1.85	0.59
1:E:23:ARG:HH22	1:E:215:GLN:NE2	2.00	0.59
1:C:557:HIS:HB2	1:C:586:VAL:HG22	1.85	0.59
1:D:466:HIS:CD2	1:D:518:ILE:HD11	2.38	0.59
1:C:77:ASP:HB3	7:C:9787:HOH:O	2.04	0.58
1:E:203:TRP:HD1	6:E:9005:PEG:H32	1.69	0.58
1:F:784:ASP:HB3	1:F:787:LEU:HD22	1.85	0.58
1:B:903[B]:MET:CE	7:B:9543:HOH:O	2.51	0.57
1:E:784:ASP:HB3	1:E:787:LEU:HD22	1.86	0.57
1:F:584:ASN:H	1:F:584:ASN:HD22	1.51	0.57
1:F:649:GLY:HA3	1:F:906[B]:ARG:HG3	1.86	0.57
1:D:690:THR:CG2	1:D:903[B]:MET:HE2	2.34	0.57
1:E:992:HIS:CD2	1:E:1009:LEU:H	2.18	0.57
1:B:227:LEU:CD1	1:B:306[A]:VAL:HG21	2.29	0.57
1:C:633:THR:HG21	7:C:9439:HOH:O	2.03	0.57
1:A:784:ASP:HB3	1:A:787:LEU:HD22	1.88	0.56
1:C:725:PRO:HG3	1:C:848:ASP:HB2	1.87	0.56
1:F:337:THR:OG1	1:F:557:HIS:HD2	1.88	0.56
1:B:948:GLU:HG2	7:B:9718:HOH:O	2.06	0.55
1:A:528:ASN:H	1:A:922:GLN:NE2	2.05	0.55
1:A:559:ILE:HD13	6:A:9001:PEG:H11	1.87	0.55
1:A:963:HIS:HD2	7:A:9655:HOH:O	1.89	0.55
1:D:259:VAL:HB	1:D:264:VAL:HG13	1.89	0.55
1:D:457:HIS:HE1	1:D:477:ASP:OD2	1.88	0.55
1:E:320:PHE:H	1:E:547:HIS:HE1	1.53	0.55
1:E:632:HIS:ND1	1:E:633:THR:CG2	2.69	0.55
1:B:337:THR:OG1	1:B:557:HIS:HD2	1.89	0.55
1:D:725:PRO:HG3	1:D:848:ASP:HB2	1.88	0.54
1:E:40[A]:ARG:HD2	1:E:78:THR:HG22	1.89	0.54
1:F:817:VAL:HG13	1:F:826:VAL:HG22	1.88	0.54
1:B:557:HIS:HB3	6:B:9002:PEG:H12	1.88	0.54
1:A:618:PRO:HG2	1:A:621:GLY:HA3	1.89	0.54
1:D:557:HIS:HB3	6:D:9004:PEG:H12	1.90	0.54
1:A:237:ALA:CB	1:A:283[B]:GLU:OE2	2.54	0.54
1:C:645:VAL:CG2	1:C:679:MET:SD	2.96	0.54
1:F:166:ARG:HG2	1:F:370:TYR:CD1	2.42	0.54
1:F:335:HIS:CD2	7:F:9706:HOH:O	2.53	0.54
1:C:337:THR:CB	1:C:557:HIS:HD2	2.21	0.53
1:D:712:GLN:HG3	1:D:903[B]:MET:CE	2.38	0.53
1:C:337:THR:OG1	1:C:557:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ARG:CZ	1:C:234:ARG:HA	2.39	0.53
1:B:205:LEU:HD11	6:B:9002:PEG:H31	1.90	0.53
1:E:557:HIS:HB2	1:E:586:VAL:HG22	1.90	0.53
1:F:512:GLN:HA	1:F:512:GLN:NE2	2.20	0.53
1:B:903[B]:MET:HE3	7:B:9543:HOH:O	2.09	0.53
1:C:227:LEU:CD1	1:C:306[B]:VAL:HG11	2.32	0.53
1:A:280:GLU:CD	1:A:280:GLU:N	2.62	0.52
1:C:222:ILE:HD13	1:C:297[B]:VAL:HG22	1.92	0.52
1:B:337:THR:CB	1:B:557:HIS:HD2	2.21	0.52
1:F:563:THR:OG1	1:F:567:MET:HB3	2.10	0.52
1:F:645[A]:VAL:CG2	1:F:679:MET:SD	2.97	0.52
1:F:557:HIS:HB2	1:F:586:VAL:HG22	1.91	0.52
1:F:710:ALA:CB	1:F:903[B]:MET:HE1	2.37	0.52
1:B:657:VAL:HG21	1:B:674:ILE:CD1	2.40	0.52
1:A:557:HIS:HB2	1:A:586:VAL:HG22	1.91	0.52
1:D:237:ALA:HB3	1:D:281:ASN:HA	1.92	0.51
1:E:319:GLN:NE2	1:E:326:ARG:HD2	2.25	0.51
1:D:581:HIS:HD2	1:D:583:SER:N	2.08	0.51
1:E:710:ALA:HB1	1:E:903[B]:MET:HE1	1.92	0.51
1:B:712:GLN:HG3	1:B:903[B]:MET:SD	2.51	0.51
1:D:642:ARG:HG2	1:D:656:GLU:HG2	1.91	0.51
1:F:645[A]:VAL:HG21	1:F:679:MET:SD	2.51	0.51
1:A:404:VAL:HG12	1:A:405[B]:GLU:HG2	1.92	0.51
1:B:457:HIS:HE1	1:B:477:ASP:OD2	1.94	0.51
1:A:674:ILE:HG13	1:A:674:ILE:O	2.10	0.51
1:A:33:LEU:HD12	1:A:35:LEU:CD1	2.40	0.50
1:B:657:VAL:HG21	1:B:674:ILE:HD11	1.93	0.50
1:A:557:HIS:HB3	6:A:9001:PEG:H12	1.94	0.50
1:B:35[A]:LEU:HD11	1:B:214:LEU:HG	1.94	0.50
1:D:96:PRO:HG2	1:D:559:ILE:HD13	1.93	0.50
1:D:632:HIS:ND1	1:D:633:THR:HG22	2.26	0.50
1:D:341:ARG:NH2	7:D:9991:HOH:O	2.44	0.50
1:B:151:LYS:HE3	1:B:158:GLU:CD	2.37	0.50
1:C:581:HIS:CD2	1:C:583:SER:H	2.18	0.50
1:B:632:HIS:ND1	1:B:633:THR:CG2	2.70	0.50
1:E:559:ILE:HD13	6:E:9005:PEG:H11	1.93	0.50
1:F:242:ILE:HB	1:F:277:LEU:HD13	1.92	0.50
1:D:929[A]:ASP:OD1	1:D:955:ARG:HD2	2.12	0.50
1:F:43:LEU:HD22	1:F:93:TYR:HB3	1.94	0.50
1:B:802:TRP:CD2	1:B:869:PRO:HG3	2.47	0.49
1:D:557:HIS:HB2	1:D:586:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:645[A]:VAL:CG2	1:E:679:MET:SD	3.00	0.49
1:F:151:LYS:HE3	1:F:158:GLU:CD	2.37	0.49
1:A:710:ALA:HB1	1:A:903[A]:MET:CE	2.42	0.49
1:B:155:ASN:HD21	1:B:182:ASN:ND2	2.08	0.49
1:F:320:PHE:H	1:F:547:HIS:HE1	1.55	0.49
1:B:644:ARG:HH11	1:B:651:VAL:HG21	1.78	0.49
1:D:545:ARG:O	1:D:547:HIS:HD2	1.95	0.49
1:E:633:THR:HG21	7:E:9044:HOH:O	2.13	0.49
1:C:581:HIS:HD2	1:C:583:SER:N	2.03	0.49
1:E:203:TRP:CD1	6:E:9005:PEG:H32	2.48	0.49
1:A:283[A]:GLU:HB2	1:A:291:ARG:HG2	1.94	0.49
1:A:295:ALA:HB3	1:A:306:VAL:HG23	1.95	0.49
1:C:674:ILE:HD11	7:C:9853:HOH:O	2.12	0.49
1:E:545:ARG:O	1:E:547:HIS:HD2	1.94	0.49
1:F:325[A]:ARG:NH1	1:F:631:ARG:O	2.45	0.48
1:B:512:GLN:HA	1:B:512:GLN:NE2	2.20	0.48
1:A:710:ALA:CB	1:A:903[A]:MET:CE	2.91	0.48
1:E:330:HIS:HE1	1:E:537:GLU:OE1	1.96	0.48
1:F:712:GLN:HG3	1:F:903[B]:MET:SD	2.53	0.48
1:A:436:MET:HE1	1:A:478:VAL:CG2	2.44	0.48
1:E:205:LEU:HD11	6:E:9005:PEG:H31	1.96	0.48
1:B:912:GLU:CD	1:B:912:GLU:H	2.22	0.48
1:A:234:ARG:O	1:A:235:SER:C	2.55	0.48
1:A:338:HIS:O	6:A:9001:PEG:H21	2.13	0.47
1:B:755:GLN:NE2	7:B:9679:HOH:O	2.47	0.47
1:A:545:ARG:O	1:A:547:HIS:HD2	1.96	0.47
1:E:272:GLU:CD	1:E:272:GLU:H	2.20	0.47
1:F:932:TRP:CZ3	1:F:934:GLU:HG3	2.49	0.47
1:A:647[B]:HIS:HD2	1:A:682:ALA:CB	2.28	0.47
1:F:666:LEU:HD22	1:F:670:GLU:HB3	1.95	0.47
1:A:320:PHE:H	1:A:547:HIS:HE1	1.53	0.47
1:D:320:PHE:H	1:D:547:HIS:HE1	1.54	0.47
1:B:545:ARG:O	1:B:547:HIS:HD2	1.97	0.47
1:C:40:ARG:HA	1:C:40:ARG:HD2	1.69	0.47
1:C:862[B]:ALA:O	7:C:9235:HOH:O	2.20	0.47
1:D:632:HIS:ND1	1:D:633:THR:CG2	2.78	0.47
1:B:633:THR:HG21	7:B:9026:HOH:O	2.14	0.47
1:D:948:GLU:HG3	7:D:9828:HOH:O	2.14	0.47
1:F:96:PRO:HB2	1:F:203:TRP:CE3	2.50	0.47
1:A:436:MET:HE2	1:A:436:MET:HB3	1.79	0.47
1:E:581:HIS:HD2	1:E:583:SER:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:679:MET:SD	1:D:689:LEU:HD13	2.54	0.46
1:C:342:GLY:HA2	6:C:9003:PEG:H22	1.96	0.46
1:A:625:LEU:HD21	1:A:641:LEU:HD13	1.98	0.46
1:C:330:HIS:HE1	1:C:537:GLU:OE1	1.98	0.46
1:F:205:LEU:HD11	6:F:9006:PEG:H31	1.97	0.46
1:D:764:LEU:O	1:D:869:PRO:HD2	2.15	0.46
1:F:330:HIS:HE1	1:F:537:GLU:OE1	1.98	0.46
1:C:553:GLU:OE1	1:C:588:ASP:OD1	2.33	0.46
1:A:36:ASN:HD21	1:A:212:VAL:H	1.63	0.46
1:F:553:GLU:OE2	1:F:557:HIS:HE1	1.98	0.46
1:F:594:ASP:O	1:F:595:SER:HB2	2.16	0.46
1:A:563:THR:OG1	1:A:567:MET:HB3	2.16	0.46
1:B:96:PRO:HB2	1:B:203:TRP:CE3	2.51	0.46
1:D:338:HIS:O	6:D:9004:PEG:H21	2.16	0.45
1:F:802:TRP:CD2	1:F:869:PRO:HG3	2.51	0.45
1:A:674:ILE:HG21	7:A:9900:HOH:O	2.16	0.45
1:D:523:VAL:HG11	1:D:533:MET:HG2	1.98	0.45
1:A:647[B]:HIS:CD2	1:A:682:ALA:CB	2.99	0.45
1:B:338:HIS:O	6:B:9002:PEG:H21	2.15	0.45
1:C:545:ARG:O	1:C:547:HIS:HD2	2.00	0.45
1:D:802:TRP:CD2	1:D:869:PRO:HG3	2.52	0.45
1:C:948:GLU:CD	1:C:949:PRO:HD2	2.42	0.45
1:F:745:ASP:C	1:F:745:ASP:OD1	2.60	0.45
1:D:283[A]:GLU:HB2	1:D:291:ARG:HG2	1.98	0.45
1:F:42:ARG:HG2	1:F:76:TRP:CH2	2.52	0.44
1:A:814:VAL:HA	1:A:828:THR:HG22	1.99	0.44
1:B:511:ARG:HG2	7:B:9863:HOH:O	2.15	0.44
1:C:438:SER:HA	1:C:466:HIS:O	2.18	0.44
1:E:937:ARG:HG2	1:E:942:TRP:CB	2.42	0.44
1:C:319:GLN:HE22	1:C:326:ARG:HD2	1.83	0.44
1:E:33:LEU:HD12	1:E:35:LEU:HD13	2.00	0.44
1:F:642:ARG:NE	1:F:656:GLU:OE1	2.37	0.44
1:D:147:GLU:HA	1:D:148[A]:SER:HA	1.84	0.44
1:C:147:GLU:HA	1:C:148[A]:SER:HA	1.57	0.44
1:F:63:VAL:HG12	1:F:64:GLU:HG3	2.00	0.44
1:F:338:HIS:O	6:F:9006:PEG:H21	2.18	0.44
1:A:25:TRP:CD2	1:A:374:PRO:HB2	2.53	0.43
1:B:584:ASN:H	1:B:584:ASN:ND2	2.09	0.43
1:B:1019[B]:ARG:HG3	7:B:9718:HOH:O	2.18	0.43
1:F:147:GLU:HA	1:F:148[A]:SER:HA	1.58	0.43
1:A:234:ARG:HG3	1:A:239:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:TRP:HD1	6:B:9002:PEG:H32	1.83	0.43
1:F:39:TRP:CE3	1:F:121:PHE:HB3	2.53	0.43
1:E:147:GLU:HA	1:E:148[B]:SER:HA	1.60	0.43
1:D:205:LEU:HD11	6:D:9004:PEG:H31	2.00	0.43
1:D:657:VAL:HG11	1:D:674:ILE:HD12	2.01	0.43
1:E:468:GLU:HG3	1:E:482[B]:MET:HG3	2.01	0.43
1:E:645[A]:VAL:HG21	1:E:679:MET:SD	2.58	0.43
1:A:237:ALA:HB3	1:A:281:ASN:HA	1.99	0.43
1:A:597:PRO:HB3	1:A:601:LEU:HD23	2.00	0.43
1:E:25:TRP:CD2	1:E:374:PRO:HB2	2.54	0.43
1:E:528:ASN:H	1:E:922:GLN:NE2	2.17	0.43
1:F:811:THR:O	1:F:830:TYR:HA	2.18	0.43
1:D:644:ARG:NH2	7:D:9704:HOH:O	2.52	0.42
1:A:147:GLU:HA	1:A:148[B]:SER:HA	1.56	0.42
1:C:166:ARG:HG2	1:C:370:TYR:CD1	2.54	0.42
1:D:227:LEU:CD1	1:D:306[A]:VAL:HG21	2.41	0.42
1:D:553:GLU:CD	1:D:557:HIS:HE2	2.26	0.42
1:A:234:ARG:HB2	1:A:238:GLY:HA2	2.01	0.42
1:F:528:ASN:H	1:F:922:GLN:NE2	2.17	0.42
1:F:553:GLU:CD	1:F:557:HIS:HE1	2.27	0.42
1:A:368:SER:HA	1:A:369:HIS:HA	1.86	0.42
1:D:24:SER:HB2	1:D:26:LEU:HG	2.02	0.42
1:E:545:ARG:O	1:E:547:HIS:CD2	2.72	0.42
1:A:337:THR:CB	1:A:557:HIS:HD1	2.32	0.42
1:A:524:HIS:CG	1:A:999:CYS:HB3	2.53	0.42
1:C:436[B]:MET:HE1	1:C:478:VAL:HG21	2.02	0.42
1:F:710:ALA:CB	1:F:903[B]:MET:CE	2.97	0.42
1:C:368:SER:HA	1:C:369:HIS:HA	1.90	0.42
1:F:368:SER:HA	1:F:369:HIS:HA	1.79	0.42
1:F:555:ARG:NH2	7:F:9526:HOH:O	2.51	0.42
1:A:768:PRO:HG2	1:A:799:GLU:HG3	2.02	0.42
1:B:147:GLU:HA	1:B:148[B]:SER:HA	1.60	0.42
1:D:784:ASP:HB3	1:D:787:LEU:HD22	2.02	0.42
1:B:958:PHE:HA	1:B:986:TYR:O	2.20	0.42
1:E:147:GLU:HA	1:E:148[A]:SER:HA	1.90	0.42
1:F:377:LEU:HD22	1:F:434:ILE:HD11	2.02	0.42
1:C:147:GLU:HA	1:C:148[B]:SER:HA	1.90	0.41
1:E:725:PRO:HG3	1:E:848:ASP:HB2	2.02	0.41
1:D:524:HIS:CG	1:D:999:CYS:HB3	2.54	0.41
1:E:773:ARG:NH1	7:E:9586:HOH:O	2.53	0.41
1:A:98:TYR:O	1:A:581:HIS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:GLN:HE21	1:E:217:ARG:HD2	1.84	0.41
1:F:286:SER:OG	1:F:633[B]:THR:HG21	2.20	0.41
1:B:338:HIS:HA	1:B:339:PRO:HD3	1.96	0.41
1:D:33:LEU:HD12	1:D:33:LEU:C	2.45	0.41
1:D:285:TRP:CH2	1:D:433:SER:HA	2.56	0.41
1:B:320:PHE:H	1:B:547:HIS:HE1	1.65	0.41
1:D:25:TRP:CD2	1:D:374:PRO:HB2	2.55	0.41
1:D:319:GLN:NE2	1:D:326:ARG:HD2	2.32	0.41
1:D:618:PRO:HG2	1:D:621:GLY:HA3	2.02	0.41
1:E:26:LEU:HD13	1:E:304:ILE:HD13	2.02	0.41
1:E:227:LEU:CD1	1:E:306:VAL:HG21	2.44	0.41
1:A:512:GLN:HA	1:A:512:GLN:NE2	2.26	0.41
1:C:524:HIS:CG	1:C:999:CYS:HB3	2.56	0.41
1:A:36:ASN:ND2	1:A:212:VAL:H	2.19	0.41
1:E:442:GLU:CD	1:E:482[B]:MET:HE1	2.45	0.41
1:A:766:ARG:HG2	1:A:869:PRO:HB3	2.03	0.41
1:D:39:TRP:CE3	1:D:121:PHE:HB3	2.56	0.41
1:D:466:HIS:HD2	1:D:518:ILE:HD11	1.82	0.41
1:E:360:PHE:CD1	1:E:601:LEU:HG	2.55	0.41
1:E:632:HIS:CE1	1:E:633:THR:HG22	2.55	0.41
1:C:944:ARG:HG3	1:C:945:ILE:N	2.36	0.41
1:D:295:ALA:HB3	1:D:306[A]:VAL:HG23	2.03	0.40
1:D:338:HIS:HA	1:D:339:PRO:HD3	1.99	0.40
1:F:4:ALA:N	7:F:9387:HOH:O	2.54	0.40
1:F:524:HIS:CG	1:F:999:CYS:HB3	2.55	0.40
1:B:43:LEU:HD22	1:B:93:TYR:HB3	2.02	0.40
1:B:553:GLU:CD	1:B:557:HIS:HE1	2.29	0.40
1:E:710:ALA:CB	1:E:903[B]:MET:HE1	2.50	0.40
1:E:764:LEU:O	1:E:869:PRO:HD2	2.22	0.40
1:A:229:THR:HG21	1:A:310:PHE:HA	2.01	0.40
1:C:466:HIS:CD2	1:C:518[B]:ILE:HD11	2.57	0.40
1:D:557:HIS:CD2	7:D:9809:HOH:O	2.74	0.40
1:B:360:PHE:CD1	1:B:601:LEU:HG	2.56	0.40
1:E:1017:LYS:HD3	7:E:9779:HOH:O	2.21	0.40
1:D:802:TRP:CE2	1:D:869:PRO:HG3	2.57	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)
7:A:9663:HOH:O	7:F:9129:HOH:O[2_545]	1.95	0.25

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1035/1024 (101%)	1005 (97%)	30 (3%)	0	100	100
1	B	1033/1024 (101%)	1004 (97%)	29 (3%)	0	100	100
1	C	1037/1024 (101%)	1006 (97%)	30 (3%)	1 (0%)	48	40
1	D	1032/1024 (101%)	1002 (97%)	30 (3%)	0	100	100
1	E	1035/1024 (101%)	1007 (97%)	28 (3%)	0	100	100
1	F	1038/1024 (101%)	1003 (97%)	35 (3%)	0	100	100
All	All	6210/6144 (101%)	6027 (97%)	182 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	523	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	815/803 (102%)	795 (98%)	20 (2%)	42	37
1	B	813/803 (101%)	794 (98%)	19 (2%)	44	40
1	C	816/803 (102%)	805 (99%)	11 (1%)	61	61
1	D	811/803 (101%)	793 (98%)	18 (2%)	45	42
1	E	816/803 (102%)	796 (98%)	20 (2%)	42	37
1	F	817/803 (102%)	803 (98%)	14 (2%)	53	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4888/4818 (102%)	4786 (98%)	102 (2%)	47 44

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	40	ARG
1	A	59[A]	SER
1	A	59[B]	SER
1	A	123	ARG
1	A	166	ARG
1	A	184	LEU
1	A	214	LEU
1	A	229	THR
1	A	232	SER
1	A	234	ARG
1	A	280	GLU
1	A	358	LYS
1	A	512	GLN
1	A	584	ASN
1	A	622	LYS
1	A	633	THR
1	A	645	VAL
1	A	666	LEU
1	A	787	LEU
1	B	33	LEU
1	B	40	ARG
1	B	79	LEU
1	B	166	ARG
1	B	264	VAL
1	B	277	LEU
1	B	297	VAL
1	B	512	GLN
1	B	584	ASN
1	B	633	THR
1	B	674	ILE
1	B	692	GLU
1	B	723	ARG
1	B	737	VAL
1	B	787	LEU
1	B	793	VAL
1	B	803	LYS

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Mol	Chain	Res	Type
1	B	933	LEU
1	B	1017	LYS
1	C	126	ASP
1	C	139	LEU
1	C	141	LEU
1	C	163	SER
1	C	166	ARG
1	C	234	ARG
1	C	235	SER
1	C	277	LEU
1	C	279	LEU
1	C	584	ASN
1	C	722	THR
1	D	40	ARG
1	D	55	SER
1	D	79	LEU
1	D	130	GLN
1	D	139	LEU
1	D	158	GLU
1	D	232	SER
1	D	264	VAL
1	D	277	LEU
1	D	279	LEU
1	D	280	GLU
1	D	633	THR
1	D	645	VAL
1	D	657	VAL
1	D	666	LEU
1	D	674	ILE
1	D	723	ARG
1	D	787	LEU
1	E	35	LEU
1	E	77	ASP
1	E	79	LEU
1	E	130	GLN
1	E	163	SER
1	E	166	ARG
1	E	214	LEU
1	E	234	ARG
1	E	272	GLU
1	E	277	LEU
1	E	279	LEU

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Mol	Chain	Res	Type
1	E	512	GLN
1	E	584	ASN
1	E	633	THR
1	E	660	GLU
1	E	773	ARG
1	E	787	LEU
1	E	804	GLN
1	E	933	LEU
1	E	979	THR
1	F	55	SER
1	F	163	SER
1	F	166	ARG
1	F	234	ARG
1	F	277	LEU
1	F	279	LEU
1	F	325[A]	ARG
1	F	325[B]	ARG
1	F	512	GLN
1	F	568	GLU
1	F	584	ASN
1	F	666	LEU
1	F	694	VAL
1	F	787	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	102	GLN
1	A	130	GLN
1	A	190	GLN
1	A	330	HIS
1	A	457	HIS
1	A	512	GLN
1	A	547	HIS
1	A	584	ASN
1	A	755	GLN
1	A	922	GLN
1	B	182	ASN
1	B	202	GLN
1	B	457	HIS
1	B	512	GLN

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Mol	Chain	Res	Type
1	B	547	HIS
1	B	557	HIS
1	B	584	ASN
1	B	755	GLN
1	C	319	GLN
1	C	330	HIS
1	C	547	HIS
1	C	557	HIS
1	C	581	HIS
1	C	584	ASN
1	C	846	GLN
1	C	982	HIS
1	D	319	GLN
1	D	330	HIS
1	D	457	HIS
1	D	498	HIS
1	D	547	HIS
1	D	581	HIS
1	D	788	ASN
1	D	982	HIS
1	E	130	GLN
1	E	215	GLN
1	E	265	ASN
1	E	319	GLN
1	E	330	HIS
1	E	457	HIS
1	E	512	GLN
1	E	547	HIS
1	E	557	HIS
1	E	581	HIS
1	E	584	ASN
1	E	755	GLN
1	E	788	ASN
1	E	922	GLN
1	E	982	HIS
1	E	992	HIS
1	F	130	GLN
1	F	202	GLN
1	F	330	HIS
1	F	335	HIS
1	F	512	GLN
1	F	547	HIS

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Mol	Chain	Res	Type
1	F	557	HIS
1	F	584	ASN
1	F	647	HIS
1	F	922	GLN
1	F	982	HIS
1	F	992	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 24 are monoatomic - leaving 17 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	$\# Z > 2$
5	SO4	F	8516	-	4,4,4	0.19	0	6,6,6	0.31	0
6	PEG	E	9005	-	6,6,6	0.73	0	5,5,5	0.62	0
5	SO4	B	8502	-	4,4,4	0.24	0	6,6,6	0.40	0
5	SO4	C	8513	-	4,4,4	0.23	0	6,6,6	0.21	0
5	SO4	E	8505	-	4,4,4	0.28	0	6,6,6	0.28	0
5	SO4	F	8506	-	4,4,4	0.27	0	6,6,6	0.33	0
6	PEG	A	9001	-	6,6,6	0.56	0	5,5,5	0.32	0
6	PEG	B	9002	-	6,6,6	0.61	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	E	8515	-	4,4,4	0.21	0	6,6,6	0.43	0
5	SO4	B	8512	-	4,4,4	0.25	0	6,6,6	0.20	0
6	PEG	C	9003	-	6,6,6	0.60	0	5,5,5	0.60	0
6	PEG	D	9004	-	6,6,6	0.56	0	5,5,5	0.39	0
6	PEG	F	9006	-	6,6,6	0.43	0	5,5,5	0.57	0
5	SO4	A	8501	-	4,4,4	0.19	0	6,6,6	0.20	0
5	SO4	D	8504	-	4,4,4	0.32	0	6,6,6	0.23	0
5	SO4	D	8514	-	4,4,4	0.23	0	6,6,6	0.30	0
5	SO4	A	8511	-	4,4,4	0.27	0	6,6,6	0.32	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
6	PEG	E	9005	-	-	2/4/4/4	-
6	PEG	A	9001	-	-	2/4/4/4	-
6	PEG	C	9003	-	-	1/4/4/4	-
6	PEG	D	9004	-	-	2/4/4/4	-
6	PEG	B	9002	-	-	2/4/4/4	-
6	PEG	F	9006	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	9005	PEG	O1-C1-C2-O2
6	A	9001	PEG	O2-C3-C4-O4
6	D	9004	PEG	O2-C3-C4-O4
6	E	9005	PEG	O2-C3-C4-O4
6	F	9006	PEG	O1-C1-C2-O2
6	F	9006	PEG	O2-C3-C4-O4
6	B	9002	PEG	O2-C3-C4-O4
6	B	9002	PEG	O1-C1-C2-O2
6	A	9001	PEG	C1-C2-O2-C3
6	C	9003	PEG	O2-C3-C4-O4
6	D	9004	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	9005	PEG	6	0
6	A	9001	PEG	3	0
6	B	9002	PEG	4	0
6	C	9003	PEG	4	0
6	D	9004	PEG	3	0
6	F	9006	PEG	3	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, 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	1020/1024 (99%)	-0.36	11 (1%) 78 80	6, 16, 30, 48	22 (2%)
1	B	1020/1024 (99%)	-0.39	12 (1%) 76 79	7, 15, 30, 49	20 (1%)
1	C	1020/1024 (99%)	-0.47	10 (0%) 79 82	7, 14, 30, 46	29 (2%)
1	D	1020/1024 (99%)	-0.45	13 (1%) 75 78	6, 15, 29, 47	21 (2%)
1	E	1020/1024 (99%)	-0.43	14 (1%) 73 76	7, 14, 29, 47	36 (3%)
1	F	1020/1024 (99%)	-0.43	13 (1%) 75 78	6, 15, 30, 45	34 (3%)
All	All	6120/6144 (99%)	-0.42	73 (1%) 76 79	6, 15, 30, 49	162 (2%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	235	SER	4.8
1	E	235	SER	4.3
1	B	235[A]	SER	4.1
1	B	720	VAL	4.1
1	A	236	GLY	4.1
1	E	564	ALA	4.0
1	E	4	ALA	4.0
1	D	235	SER	4.0
1	F	237	ALA	3.9
1	E	938	ALA	3.8
1	A	235	SER	3.8
1	C	236	GLY	3.8
1	E	720	VAL	3.6
1	F	4	ALA	3.5
1	E	236	GLY	3.5
1	E	620	GLY	3.5
1	B	236[A]	GLY	3.5
1	C	237	ALA	3.4
1	E	237	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	721	PRO	3.3
1	A	720	VAL	3.3
1	B	721	PRO	3.3
1	F	236	GLY	3.2
1	D	564	ALA	3.2
1	C	235	SER	3.1
1	E	722	THR	3.0
1	F	564	ALA	3.0
1	A	732	ASP	2.9
1	E	721	PRO	2.9
1	A	237	ALA	2.9
1	B	564	ALA	2.9
1	B	719	ALA	2.9
1	B	939	GLY	2.9
1	D	53	ALA	2.8
1	F	720	VAL	2.8
1	F	567	MET	2.7
1	A	4	ALA	2.7
1	D	720	VAL	2.7
1	D	234	ARG	2.6
1	F	721	PRO	2.6
1	C	564	ALA	2.6
1	A	563	THR	2.6
1	F	1023	ALA	2.6
1	B	4	ALA	2.5
1	C	1023	ALA	2.4
1	A	234	ARG	2.4
1	D	722	THR	2.4
1	A	564	ALA	2.4
1	C	619	ALA	2.4
1	A	731	LEU	2.3
1	C	850	GLY	2.2
1	D	237	ALA	2.2
1	D	849	GLY	2.2
1	D	236	GLY	2.1
1	F	732	ASP	2.1
1	F	822	ASP	2.1
1	B	621	GLY	2.1
1	C	723	ARG	2.1
1	C	849	GLY	2.1
1	D	4	ALA	2.1
1	F	619	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	619	ALA	2.1
1	D	732	ASP	2.1
1	B	849	GLY	2.0
1	D	939	GLY	2.0
1	E	733	GLY	2.0
1	C	721	PRO	2.0
1	B	723	ARG	2.0
1	E	234	ARG	2.0
1	E	723	ARG	2.0
1	E	59	SER	2.0
1	D	620	GLY	2.0
1	F	620	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	A	9001	7/7	0.81	0.18	38,39,41,41	0
6	PEG	C	9003	7/7	0.82	0.18	28,30,33,36	0
6	PEG	E	9005	7/7	0.83	0.16	28,29,33,33	0
5	SO4	D	8504	5/5	0.84	0.14	54,55,55,56	0
5	SO4	C	8513	5/5	0.86	0.20	37,38,40,40	5
5	SO4	E	8515	5/5	0.86	0.18	26,26,29,29	5
5	SO4	F	8516	5/5	0.86	0.22	33,33,36,36	5
6	PEG	F	9006	7/7	0.86	0.14	31,35,36,37	0
3	NA	B	7502	1/1	0.87	0.17	44,44,44,44	0
5	SO4	B	8512	5/5	0.88	0.18	30,30,32,32	5
5	SO4	A	8511	5/5	0.88	0.15	23,25,27,28	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	B	9002	7/7	0.88	0.15	28,32,33,34	0
3	NA	D	7504	1/1	0.89	0.23	39,39,39,39	0
6	PEG	D	9004	7/7	0.89	0.12	31,33,35,35	0
5	SO4	D	8514	5/5	0.90	0.14	31,31,32,32	5
5	SO4	F	8506	5/5	0.91	0.12	34,34,35,35	5
5	SO4	E	8505	5/5	0.92	0.14	40,41,42,43	0
5	SO4	A	8501	5/5	0.94	0.11	29,30,31,31	5
3	NA	C	7503	1/1	0.94	0.12	41,41,41,41	0
5	SO4	B	8502	5/5	0.95	0.15	30,30,32,33	0
3	NA	E	7505	1/1	0.95	0.20	38,38,38,38	0
3	NA	F	7506	1/1	0.95	0.22	47,47,47,47	0
3	NA	A	7501	1/1	0.96	0.20	38,38,38,38	0
3	NA	D	7514	1/1	0.97	0.10	30,30,30,30	0
3	NA	C	7513	1/1	0.97	0.11	29,29,29,29	0
3	NA	B	7512	1/1	0.98	0.07	32,32,32,32	0
3	NA	F	7516	1/1	0.98	0.12	33,33,33,33	0
4	CL	A	8011	1/1	0.98	0.07	30,30,30,30	0
4	CL	F	8016	1/1	0.98	0.05	32,32,32,32	0
3	NA	A	7511	1/1	0.98	0.08	30,30,30,30	0
2	MG	C	7003	1/1	0.98	0.08	19,19,19,19	0
3	NA	E	7515	1/1	0.98	0.14	31,31,31,31	0
2	MG	E	7005	1/1	0.99	0.06	15,15,15,15	0
2	MG	F	7006	1/1	0.99	0.07	17,17,17,17	0
2	MG	B	7002	1/1	0.99	0.09	18,18,18,18	0
2	MG	A	7001	1/1	0.99	0.07	17,17,17,17	0
2	MG	D	7004	1/1	0.99	0.03	20,20,20,20	0
4	CL	B	8012	1/1	0.99	0.05	27,27,27,27	0
4	CL	C	8013	1/1	0.99	0.04	30,30,30,30	0
4	CL	D	8014	1/1	0.99	0.03	28,28,28,28	0
4	CL	E	8015	1/1	0.99	0.03	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.