



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:58 AM UTC

PDB ID : 7ZB1 / pdb_00007zb1
Title : S580A with 18mer
Authors : Song, H.; Naismith, J.H.
Deposited on : 2022-03-23
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

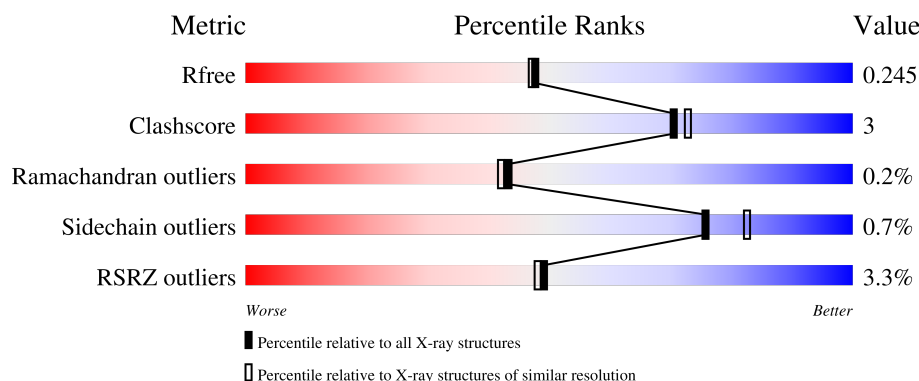
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	745	 3% 87% 9% .
1	B	745	 3% 89% 8% .
1	C	745	 3% 89% 7% .
1	D	745	 3% 90% 7% .
2	E	18	 11% 6% 28% 6% 61%

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Mol	Chain	Length	Quality of chain
2	F	18	6%28%11%61%
2	G	18	6%22%11%61%
2	H	18	11%11%11%67%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24127 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.

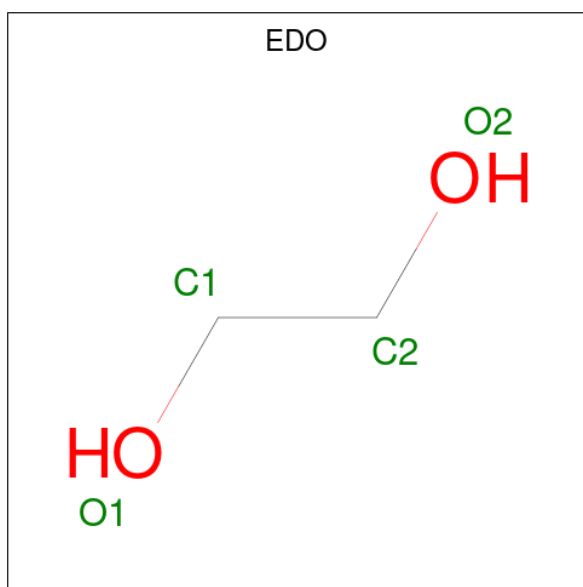
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	1	0
			5771	3689	970	1086	26			
1	B	725	Total	C	N	O	S	0	1	0
			5813	3710	979	1097	27			
1	C	721	Total	C	N	O	S	0	2	0
			5794	3700	977	1091	26			
1	D	724	Total	C	N	O	S	0	3	0
			5826	3718	980	1101	27			

- Molecule 2 is a protein called 18mer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	0	0	0
			49	34	7	8			
2	F	7	Total	C	N	O	0	0	0
			49	34	7	8			
2	G	7	Total	C	N	O	0	0	0
			49	34	7	8			
2	H	6	Total	C	N	O	0	0	0
			40	27	6	7			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

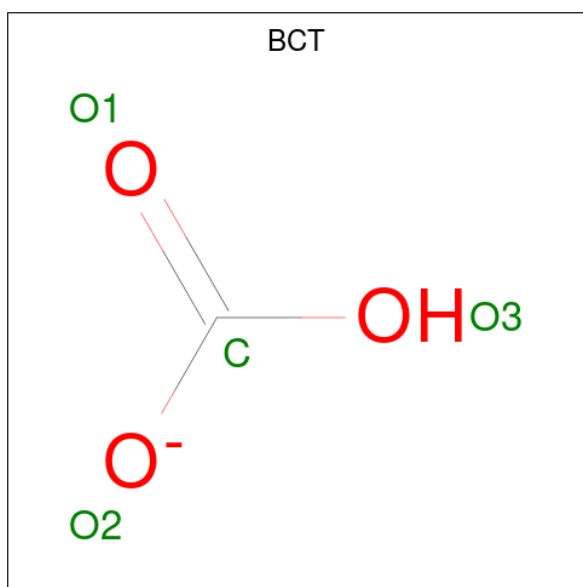


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

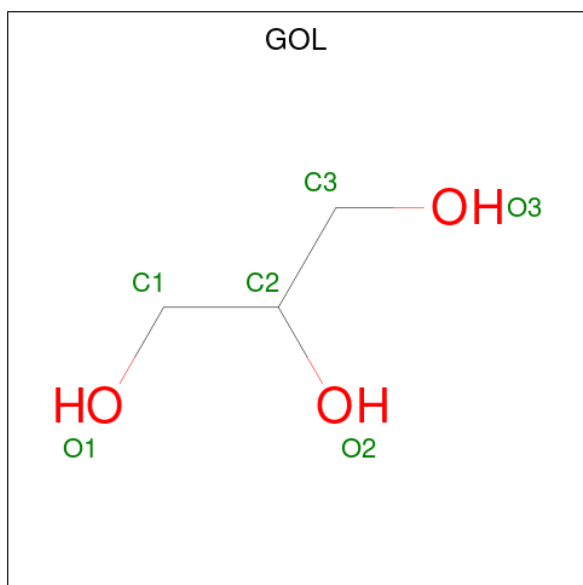
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	Na	0	0
			6	6		
4	B	4	Total	Na	0	0
			4	4		
4	C	3	Total	Na	0	0
			3	3		
4	D	3	Total	Na	0	0
			3	3		

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

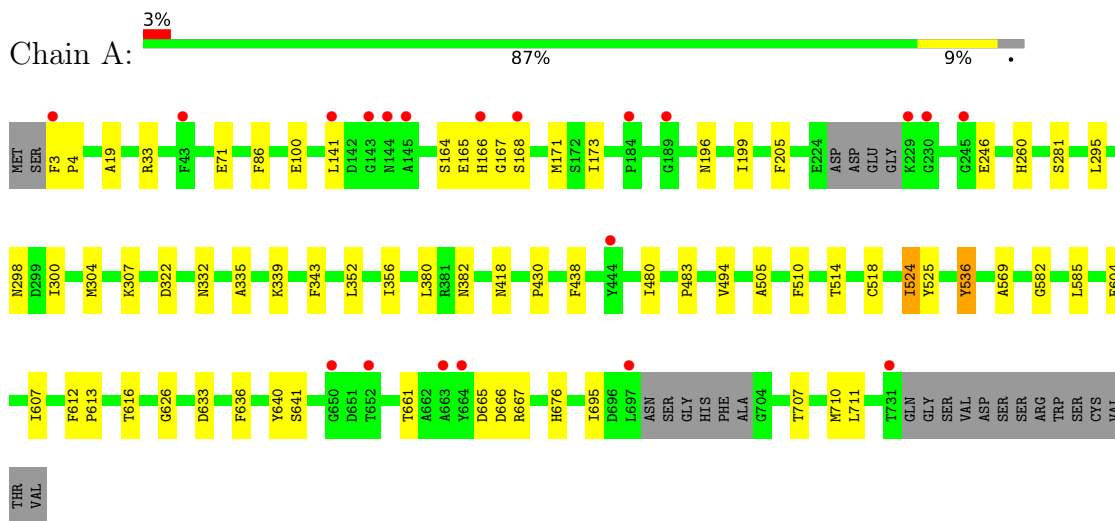
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	192	Total	O	0	0
			192	192		
7	B	121	Total	O	0	0
			121	121		
7	C	155	Total	O	0	0
			155	155		
7	D	214	Total	O	0	0
			214	214		

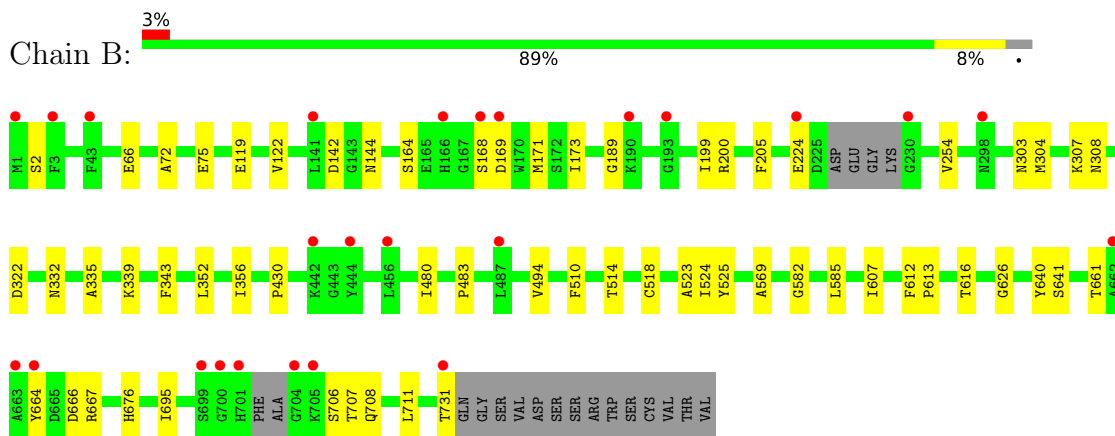
3 Residue-property plots

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

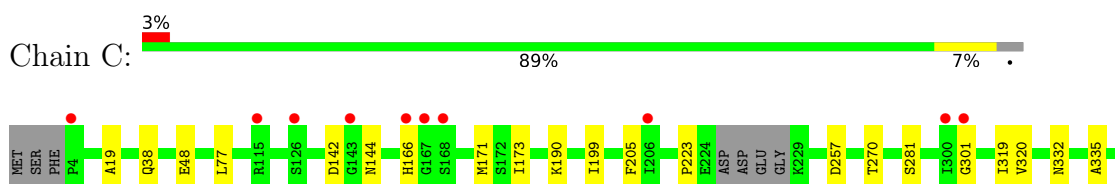
• Molecule 1: Prolyl endopeptidase

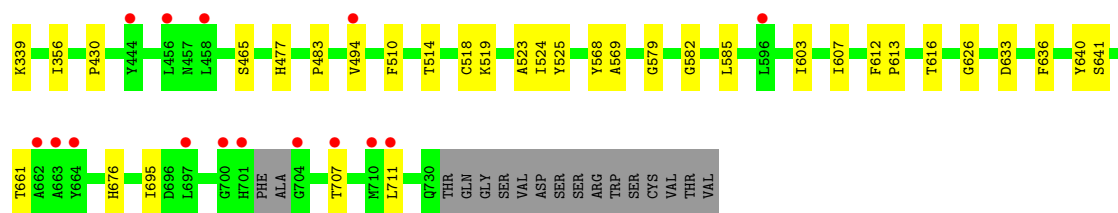


• Molecule 1: Prolyl endopeptidase

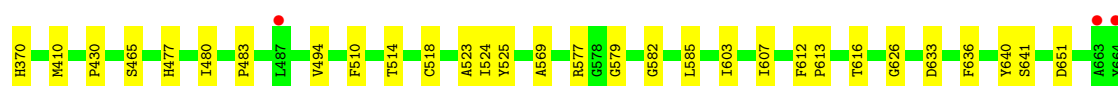
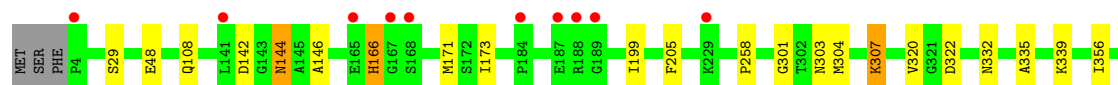
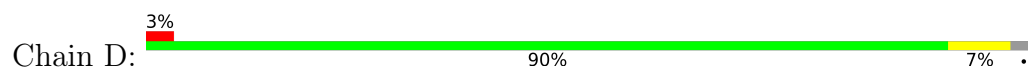


• Molecule 1: Prolyl endopeptidase

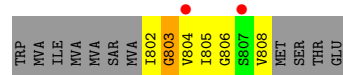
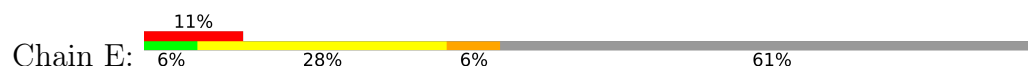




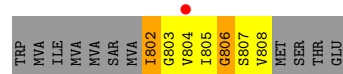
● Molecule 1: Prolyl endopeptidase



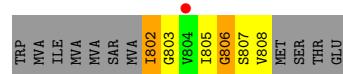
● Molecule 2: 18mer



● Molecule 2: 18mer



● Molecule 2: 18mer



● Molecule 2: 18mer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.01Å 104.61Å 110.65Å 115.81° 98.87° 93.79°	Depositor
Resolution (Å)	55.84 – 2.00 55.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (55.84-2.00) 97.9 (55.84-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.238 0.213 , 0.245	Depositor DCC
R_{free} test set	9445 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	1.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24127	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MVA, IML, SAR, NA, EDO, BCT, GOL

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	1.02	1/5939 (0.0%)	1.30	3/8055 (0.0%)
1	B	1.00	0/5982	1.30	5/8113 (0.1%)
1	C	1.02	0/5963	1.30	4/8086 (0.0%)
1	D	1.06	3/5996 (0.1%)	1.30	2/8132 (0.0%)
2	E	0.83	0/11	0.60	0/12
2	F	0.80	0/11	0.62	0/12
2	G	0.83	0/11	0.61	0/12
2	H	0.85	0/11	0.54	0/12
All	All	1.03	4/23924 (0.0%)	1.30	14/32434 (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
2	E	0	1
2	F	0	1
2	G	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	HIS	CE1-NE2	6.55	1.39	1.32
1	D	307	LYS	C-O	6.32	1.31	1.23
1	D	651	ASP	C-O	5.26	1.29	1.24
1	D	370	HIS	CE1-NE2	5.17	1.37	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	626	GLY	CA-C-O	-6.90	117.07	122.52
1	C	301	GLY	CA-C-O	-6.53	116.41	120.91
1	B	626	GLY	CA-C-O	-6.35	117.50	122.52
1	C	626	GLY	CA-C-O	-6.34	117.51	122.52
1	A	626	GLY	CA-C-O	-5.81	117.93	122.52
1	B	308	ASN	CA-C-N	5.61	128.07	120.44
1	B	308	ASN	C-N-CA	5.61	128.07	120.44
1	B	731	THR	CA-C-O	5.37	129.93	120.80
1	B	322	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	322	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	77	LEU	CA-C-N	5.10	127.07	120.44
1	C	77	LEU	C-N-CA	5.10	127.07	120.44
1	A	322	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	536	TYR	CB-CA-C	5.00	119.18	111.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	802	IML	Peptide
2	F	802	IML	Peptide
2	G	802	IML	Peptide

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	5771	0	5520	44	0
1	B	5813	0	5548	37	0
1	C	5794	0	5532	37	0
1	D	5826	0	5557	35	0
2	E	49	0	62	2	0
2	F	49	0	62	7	0
2	G	49	0	62	4	0
2	H	40	0	49	2	0
3	A	4	0	6	2	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	0	0	0
4	B	4	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	C	4	0	0	0	0
5	D	12	0	0	0	0
6	C	6	0	8	1	0
7	A	192	0	0	1	0
7	B	121	0	0	1	0
7	C	155	0	0	2	0
7	D	214	0	0	1	0
All	All	24127	0	22424	158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:VAL:HG22	1:A:524:ILE:HG12	1.66	0.76
1:A:246:GLU:OE1	1:B:189:GLY:O	2.04	0.75
1:C:494:VAL:HG22	1:C:524:ILE:HG12	1.69	0.74
1:A:418:ASN:ND2	1:A:438:PHE:O	2.29	0.66
1:A:514[A]:THR:HG21	1:A:525:TYR:CG	2.31	0.66
1:C:281:SER:OG	2:G:803:SAR:HN3	1.95	0.65
1:C:514:THR:HG21	1:C:525:TYR:CG	2.33	0.64
1:D:108:GLN:HE22	1:D:146:ALA:HA	1.63	0.63
1:B:494:VAL:CG2	1:B:569:ALA:HB2	2.29	0.63
1:B:514:THR:HG21	1:B:525:TYR:CD2	2.35	0.62
1:A:514[A]:THR:HG21	1:A:525:TYR:CD2	2.35	0.61
2:F:802:IML:N	2:F:803:SAR:HN1	2.15	0.61
1:A:3:PHE:CD1	1:A:4:PRO:HD2	2.36	0.60
1:A:71:GLU:HG3	1:C:190:LYS:HG2	1.82	0.60
1:B:514:THR:HG21	1:B:525:TYR:CG	2.36	0.60
1:C:257:ASP:OD1	7:C:901:HOH:O	2.16	0.60
1:C:514:THR:HG21	1:C:525:TYR:CD2	2.36	0.59
1:C:494:VAL:CG2	1:C:569:ALA:HB2	2.33	0.58
1:A:380:LEU:HD21	1:A:505:ALA:HB2	1.86	0.58
1:D:480:ILE:HG23	1:D:524:ILE:CG2	2.34	0.58
1:D:494:VAL:CG2	1:D:569:ALA:HB2	2.34	0.57
1:B:494:VAL:HG23	1:B:569:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:VAL:HG22	1:A:524:ILE:CG1	2.35	0.56
1:C:257:ASP:HB3	6:C:803:GOL:H2	1.89	0.55
1:A:166:HIS:C	1:A:168:SER:H	2.15	0.55
1:D:144:ASN:OD1	1:D:144:ASN:C	2.50	0.54
1:D:514:THR:HG21	1:D:525:TYR:CG	2.42	0.54
1:A:514[A]:THR:HG21	1:A:525:TYR:CD1	2.43	0.54
1:B:303:ASN:OD1	1:C:19:ALA:O	2.26	0.53
1:D:142:ASP:OD1	1:D:144:ASN:ND2	2.35	0.53
1:C:494:VAL:HG22	1:C:524:ILE:CG1	2.37	0.53
1:A:604:GLU:HG3	1:A:665:ASP:OD2	2.08	0.52
1:D:514:THR:HG21	1:D:525:TYR:CD2	2.44	0.52
1:C:514:THR:HG21	1:C:525:TYR:CD1	2.44	0.52
2:F:802:IML:N	2:F:803:SAR:CN	2.73	0.52
1:A:281:SER:OG	2:E:803:SAR:HN3	2.09	0.51
1:B:706:SER:OG	1:B:708:GLN:HG2	2.10	0.51
1:A:382:ASN:HA	1:A:536:TYR:CE1	2.46	0.51
1:B:494:VAL:HG23	1:B:569:ALA:CB	2.41	0.51
1:B:169:ASP:HB2	1:B:666:ASP:HB2	1.92	0.50
1:C:142:ASP:HB3	1:C:144:ASN:HD22	1.77	0.49
1:C:465:SER:OG	1:C:477:HIS:NE2	2.46	0.49
1:B:612:PHE:CG	1:B:613:PRO:HD3	2.48	0.49
1:D:612:PHE:CG	1:D:613:PRO:HD3	2.47	0.49
1:B:480:ILE:HG23	1:B:524:ILE:CG2	2.42	0.49
1:A:171:MET:HE1	1:A:205:PHE:HD1	1.78	0.49
1:A:307:LYS:HE2	1:D:29:SER:OG	2.11	0.49
1:C:612:PHE:CG	1:C:613:PRO:HD3	2.47	0.49
1:A:494:VAL:CG2	1:A:569:ALA:HB2	2.43	0.48
1:B:66:GLU:HG2	1:D:166:HIS:CD2	2.49	0.48
1:A:480:ILE:HG23	1:A:524:ILE:HD12	1.96	0.47
1:A:612:PHE:CG	1:A:613:PRO:HD3	2.49	0.47
2:F:804:VAL:HA	2:F:805:IML:HN1	1.67	0.47
1:C:707:THR:O	1:C:711:LEU:HG	2.15	0.47
1:A:707:THR:O	1:A:711:LEU:HG	2.15	0.47
1:A:607:ILE:HG21	1:A:676:HIS:CG	2.50	0.47
1:B:430:PRO:HA	1:B:510:PHE:CG	2.50	0.47
1:D:707:THR:O	1:D:711:LEU:HG	2.15	0.47
1:C:494:VAL:HG23	1:C:569:ALA:CB	2.45	0.47
1:A:339:LYS:HB2	1:A:356:ILE:O	2.15	0.47
1:D:171[A]:MET:HE1	1:D:205:PHE:HB2	1.97	0.47
1:B:171:MET:HE1	1:B:205:PHE:HD1	1.79	0.46
1:C:430:PRO:HA	1:C:510:PHE:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:VAL:HG23	1:D:569:ALA:CB	2.46	0.46
1:B:607:ILE:HG21	1:B:676:HIS:CG	2.50	0.46
1:C:607:ILE:HG21	1:C:676:HIS:CG	2.51	0.46
1:D:518:CYS:HA	1:D:523:ALA:HB3	1.97	0.46
1:C:171:MET:HE1	1:C:205:PHE:HD1	1.81	0.46
1:D:430:PRO:HA	1:D:510:PHE:CG	2.51	0.46
1:D:301:GLY:H	1:D:304:MET:HE2	1.81	0.46
1:D:483:PRO:HD3	1:D:518:CYS:HB3	1.97	0.46
2:H:804:VAL:HA	2:H:805:IML:HN1	1.66	0.46
3:A:801:EDO:H11	1:D:258:PRO:HG2	1.98	0.45
1:D:607:ILE:HG21	1:D:676:HIS:CG	2.51	0.45
2:F:807:SER:HA	2:F:808:MVA:HN1	1.74	0.45
1:A:196:ASN:OD1	1:B:200:ARG:HD2	2.16	0.45
1:A:514[A]:THR:CG2	1:A:525:TYR:CG	2.99	0.45
1:B:483:PRO:HD3	1:B:518:CYS:HB3	1.98	0.45
1:B:514:THR:HG21	1:B:525:TYR:CD1	2.52	0.45
1:B:707:THR:O	1:B:711:LEU:HG	2.17	0.45
1:A:640:TYR:O	1:A:641:SER:C	2.60	0.45
1:B:514:THR:CG2	1:B:525:TYR:CG	3.00	0.45
1:A:430:PRO:HA	1:A:510:PHE:CG	2.51	0.45
1:A:19:ALA:H	1:D:303:ASN:HD21	1.64	0.45
1:A:141:LEU:HD22	1:C:223:PRO:HB3	1.99	0.45
1:A:380:LEU:HD21	1:A:505:ALA:CB	2.46	0.45
1:D:514:THR:HG21	1:D:525:TYR:CD1	2.52	0.45
1:B:339:LYS:HB2	1:B:356:ILE:O	2.16	0.45
1:D:494:VAL:HG23	1:D:569:ALA:HB2	1.99	0.45
1:A:298:ASN:HB3	1:A:304:MET:HG2	1.98	0.45
1:B:303:ASN:HB3	7:B:924:HOH:O	2.16	0.45
1:B:582:GLY:O	1:B:585:LEU:HB3	2.17	0.45
1:D:640:TYR:O	1:D:641:SER:C	2.60	0.45
3:A:801:EDO:C1	1:D:258:PRO:HG2	2.48	0.44
1:C:494:VAL:HG23	1:C:569:ALA:HB2	1.99	0.44
2:G:802:IML:HG13	2:G:803:SAR:HN1	1.98	0.44
1:B:640:TYR:O	1:B:641:SER:C	2.60	0.44
1:C:640:TYR:O	1:C:641:SER:C	2.61	0.44
2:E:804:VAL:HA	2:E:805:IML:HN1	1.69	0.44
2:F:805:IML:HA	2:F:806:SAR:HN1	1.85	0.44
1:A:332:ASN:HA	1:A:335:ALA:O	2.18	0.44
2:F:802:IML:O	2:F:802:IML:HG22	2.17	0.44
1:A:483:PRO:HD3	1:A:518:CYS:HB3	1.99	0.43
1:C:582:GLY:O	1:C:585:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ASN:HA	1:D:335:ALA:O	2.18	0.43
1:C:514:THR:CG2	1:C:525:TYR:CG	3.00	0.43
1:D:582:GLY:O	1:D:585:LEU:HB3	2.19	0.43
1:A:166:HIS:O	1:A:168:SER:N	2.49	0.43
1:C:48:GLU:HG2	7:C:1042:HOH:O	2.17	0.43
1:C:171:MET:HE1	1:C:205:PHE:HB2	2.00	0.43
1:C:339:LYS:HB2	1:C:356:ILE:O	2.19	0.43
1:A:582:GLY:O	1:A:585:LEU:HB3	2.18	0.43
1:C:173:ILE:HB	1:C:199:ILE:HB	2.00	0.43
1:D:577:ARG:NH2	7:D:911:HOH:O	2.51	0.43
2:H:805:IML:HA	2:H:806:SAR:HN1	1.87	0.43
1:D:410:MET:HE3	1:D:410:MET:HB2	1.83	0.43
1:B:164:SER:HB2	1:B:168:SER:O	2.19	0.43
1:B:173:ILE:HB	1:B:199:ILE:HB	2.01	0.43
1:B:518:CYS:HA	1:B:523:ALA:HB3	2.00	0.43
1:C:332:ASN:HA	1:C:335:ALA:O	2.20	0.42
1:C:633:ASP:HA	1:C:636:PHE:CE2	2.54	0.42
1:D:339:LYS:HB2	1:D:356:ILE:O	2.20	0.42
1:B:72:ALA:O	1:B:75:GLU:HG2	2.20	0.42
2:G:807:SER:HA	2:G:808:MVA:HN1	1.77	0.42
1:A:295:LEU:HD22	1:A:300:ILE:CD1	2.50	0.42
1:A:604:GLU:CG	1:A:665:ASP:OD2	2.68	0.42
1:B:664:TYR:CD1	1:B:664:TYR:O	2.72	0.42
1:D:514:THR:CG2	1:D:525:TYR:CG	3.03	0.42
1:B:661:THR:O	1:B:695:ILE:HA	2.20	0.42
1:A:86:PHE:HA	1:A:100:GLU:O	2.19	0.41
1:C:38:GLN:O	1:C:38:GLN:NE2	2.53	0.41
1:C:483:PRO:HD3	1:C:518:CYS:HB3	2.01	0.41
1:C:518:CYS:HA	1:C:523:ALA:HB3	2.02	0.41
1:B:332:ASN:HA	1:B:335:ALA:O	2.20	0.41
1:D:480:ILE:HG23	1:D:524:ILE:HG23	2.01	0.41
1:A:514[A]:THR:HG21	1:A:525:TYR:CE2	2.56	0.41
1:B:343:PHE:HB2	1:B:352:LEU:CD1	2.51	0.41
1:C:661:THR:O	1:C:695:ILE:HA	2.21	0.41
1:C:524:ILE:HD13	1:C:568:TYR:HB3	2.02	0.41
1:D:173:ILE:HB	1:D:199:ILE:HB	2.02	0.41
1:D:579:GLY:HA2	1:D:603:ILE:O	2.20	0.41
2:G:805:IML:HA	2:G:806:SAR:HN1	1.88	0.41
1:A:633:ASP:HA	1:A:636:PHE:CE2	2.55	0.41
1:A:710:MET:HE2	7:A:949:HOH:O	2.19	0.41
1:D:465:SER:OG	1:D:477:HIS:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:ASP:HA	1:D:636:PHE:CE2	2.55	0.41
2:F:802:IML:HN2	2:F:802:IML:HB	1.84	0.41
1:B:514:THR:HG21	1:B:525:TYR:CE2	2.56	0.41
1:C:270:THR:HA	1:C:319:ILE:HG21	2.03	0.41
1:A:661:THR:O	1:A:695:ILE:HA	2.20	0.40
1:C:579:GLY:HA2	1:C:603:ILE:O	2.20	0.40
1:A:173:ILE:HB	1:A:199:ILE:HB	2.03	0.40
1:B:119:GLU:O	1:B:122:VAL:HG22	2.20	0.40
1:B:171:MET:HE1	1:B:205:PHE:HB2	2.03	0.40
1:B:254:VAL:HG13	1:B:304:MET:HE3	2.03	0.40
1:A:164:SER:HB2	1:A:168:SER:O	2.22	0.40
1:A:343:PHE:HB2	1:A:352:LEU:CD1	2.52	0.40
1:B:142:ASP:CG	1:B:144:ASN:HD22	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	714/745 (96%)	688 (96%)	24 (3%)	2 (0%)	36	35
1	B	720/745 (97%)	697 (97%)	21 (3%)	2 (0%)	36	35
1	C	717/745 (96%)	691 (96%)	25 (4%)	1 (0%)	48	46
1	D	723/745 (97%)	697 (96%)	24 (3%)	2 (0%)	36	35
2	E	2/18 (11%)	2 (100%)	0	0	100	100
2	F	2/18 (11%)	2 (100%)	0	0	100	100
2	G	2/18 (11%)	2 (100%)	0	0	100	100
2	H	2/18 (11%)	2 (100%)	0	0	100	100
All	All	2882/3052 (94%)	2781 (96%)	94 (3%)	7 (0%)	43	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	GLY
1	B	2	SER
1	D	616	THR
1	A	616	THR
1	B	616	THR
1	C	616	THR
1	D	166	HIS

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	623/644 (97%)	618 (99%)	5 (1%)	73	80
1	B	628/644 (98%)	625 (100%)	3 (0%)	81	87
1	C	625/644 (97%)	622 (100%)	3 (0%)	81	87
1	D	629/644 (98%)	623 (99%)	6 (1%)	68	75
2	E	2/8 (25%)	2 (100%)	0	100	100
2	F	2/8 (25%)	2 (100%)	0	100	100
2	G	2/8 (25%)	2 (100%)	0	100	100
2	H	2/8 (25%)	2 (100%)	0	100	100
All	All	2513/2608 (96%)	2496 (99%)	17 (1%)	76	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	165	GLU
1	A	524	ILE
1	A	666	ASP
1	A	667	ARG
1	B	224	GLU
1	B	307	LYS

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Mol	Chain	Res	Type
1	B	667	ARG
1	C	166	HIS
1	C	320	VAL
1	C	519	LYS
1	D	48	GLU
1	D	144	ASN
1	D	307	LYS
1	D	320	VAL
1	D	666	ASP
1	D	701	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	683	ASN
1	B	108	GLN
1	B	144	ASN
1	B	683	ASN
1	C	108	GLN
1	C	144	ASN
1	C	708	GLN
1	D	108	GLN
1	D	303	ASN
1	D	550	GLN
1	D	592	GLN
1	D	683	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

19 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IML	G	805	2	7,8,9	0.51	0	6,9,11	0.90	0
2	IML	F	802	2	7,8,9	0.49	0	6,9,11	0.93	0
2	SAR	G	803	2	3,4,5	0.84	0	1,3,5	1.97	0
2	SAR	F	806	2	3,4,5	0.86	0	1,3,5	2.05	1 (100%)
2	IML	G	802	2	7,8,9	0.46	0	6,9,11	0.85	0
2	SAR	G	806	2	3,4,5	0.88	0	1,3,5	2.28	1 (100%)
2	MVA	G	808	2	6,7,8	0.63	0	6,8,10	0.92	0
2	SAR	H	803	2	3,4,5	0.79	0	1,3,5	2.14	1 (100%)
2	SAR	H	806	2	3,4,5	0.92	0	1,3,5	2.18	1 (100%)
2	MVA	F	808	2	6,7,8	0.62	0	6,8,10	0.90	0
2	IML	E	805	2	7,8,9	0.48	0	6,9,11	0.85	0
2	MVA	H	808	2	6,7,8	0.74	0	6,8,10	0.98	0
2	IML	H	805	2	7,8,9	0.51	0	6,9,11	0.95	1 (16%)
2	IML	F	805	2	7,8,9	0.56	0	6,9,11	0.85	0
2	IML	E	802	2	7,8,9	0.42	0	6,9,11	1.07	0
2	SAR	E	806	2	3,4,5	0.92	0	1,3,5	2.24	1 (100%)
2	SAR	F	803	2	3,4,5	0.77	0	1,3,5	1.93	0
2	SAR	E	803	2	3,4,5	0.86	0	1,3,5	2.01	1 (100%)
2	MVA	E	808	2	6,7,8	0.59	0	6,8,10	1.05	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IML	G	805	2	-	1/8/10/12	-
2	IML	F	802	2	-	6/8/10/12	-
2	SAR	G	803	2	-	1/1/2/3	-
2	SAR	F	806	2	-	1/1/2/3	-
2	IML	G	802	2	-	6/8/10/12	-
2	SAR	G	806	2	-	1/1/2/3	-
2	MVA	G	808	2	-	2/6/8/10	-
2	SAR	H	803	2	-	1/1/2/3	-
2	SAR	H	806	2	-	1/1/2/3	-
2	MVA	F	808	2	-	1/6/8/10	-
2	IML	E	805	2	-	1/8/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MVA	H	808	2	-	5/6/8/10	-
2	IML	H	805	2	-	2/8/10/12	-
2	IML	F	805	2	-	2/8/10/12	-
2	IML	E	802	2	-	7/8/10/12	-
2	SAR	E	806	2	-	1/1/2/3	-
2	SAR	F	803	2	-	1/1/2/3	-
2	SAR	E	803	2	-	1/1/2/3	-
2	MVA	E	808	2	-	5/6/8/10	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	806	SAR	O-C-CA	-2.28	117.31	125.17
2	E	806	SAR	O-C-CA	-2.24	117.46	125.17
2	E	808	MVA	O-C-CA	-2.19	119.07	124.86
2	H	806	SAR	O-C-CA	-2.18	117.67	125.17
2	H	803	SAR	O-C-CA	-2.14	117.82	125.17
2	F	806	SAR	O-C-CA	-2.05	118.11	125.17
2	H	805	IML	O-C-CA	-2.05	119.43	124.86
2	E	803	SAR	O-C-CA	-2.01	118.26	125.17

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	802	IML	CB-CA-N-CN
2	E	802	IML	N-CA-CB-CG2
2	E	802	IML	C-CA-CB-CG2
2	E	802	IML	C-CA-CB-CG1
2	F	802	IML	CB-CA-N-CN
2	F	802	IML	N-CA-CB-CG2
2	F	802	IML	N-CA-CB-CG1
2	F	802	IML	C-CA-CB-CG2
2	F	802	IML	C-CA-CB-CG1
2	G	802	IML	N-CA-CB-CG1
2	G	802	IML	C-CA-CB-CG2
2	G	802	IML	C-CA-CB-CG1
2	E	803	SAR	C-CA-N-CN
2	F	803	SAR	C-CA-N-CN

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Mol	Chain	Res	Type	Atoms
2	G	803	SAR	C-CA-N-CN
2	H	803	SAR	C-CA-N-CN
2	F	805	IML	O-C-CA-CB
2	H	805	IML	O-C-CA-CB
2	E	806	SAR	C-CA-N-CN
2	F	806	SAR	C-CA-N-CN
2	G	806	SAR	C-CA-N-CN
2	H	806	SAR	C-CA-N-CN
2	E	808	MVA	CB-CA-N-CN
2	E	808	MVA	N-CA-CB-CG1
2	E	808	MVA	N-CA-CB-CG2
2	E	808	MVA	C-CA-CB-CG1
2	E	808	MVA	C-CA-CB-CG2
2	F	808	MVA	CB-CA-N-CN
2	H	808	MVA	CB-CA-N-CN
2	H	808	MVA	N-CA-CB-CG1
2	H	808	MVA	N-CA-CB-CG2
2	H	808	MVA	C-CA-CB-CG1
2	H	808	MVA	C-CA-CB-CG2
2	G	802	IML	N-CA-CB-CG2
2	E	802	IML	N-CA-CB-CG1
2	E	802	IML	CG2-CB-CG1-CD1
2	E	802	IML	CA-CB-CG1-CD1
2	F	802	IML	O-C-CA-CB
2	E	805	IML	CB-CA-N-CN
2	F	805	IML	CB-CA-N-CN
2	G	805	IML	CB-CA-N-CN
2	H	805	IML	CB-CA-N-CN
2	G	808	MVA	CB-CA-N-CN
2	G	802	IML	CA-CB-CG1-CD1
2	G	808	MVA	N-CA-CB-CG1
2	G	802	IML	CG2-CB-CG1-CD1

There are no ring outliers.

14 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	805	IML	1	0
2	F	802	IML	4	0
2	G	803	SAR	2	0
2	F	806	SAR	1	0
2	G	802	IML	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	806	SAR	1	0
2	G	808	MVA	1	0
2	H	806	SAR	1	0
2	F	808	MVA	1	0
2	E	805	IML	1	0
2	H	805	IML	2	0
2	F	805	IML	2	0
2	F	803	SAR	2	0
2	E	803	SAR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 16 are monoatomic - leaving 9 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	EDO	C	801	-	3,3,3	0.07	0	2,2,2	0.12	0
5	BCT	D	801	-	3,3,3	1.47	0	2,3,3	0.79	0
5	BCT	C	802	-	3,3,3	1.41	0	2,3,3	0.94	0
6	GOL	C	803	-	5,5,5	0.11	0	5,5,5	0.41	0
3	EDO	D	802	-	3,3,3	0.04	0	2,2,2	0.12	0
3	EDO	A	801	-	3,3,3	0.15	0	2,2,2	0.27	0
5	BCT	D	804	-	3,3,3	1.46	0	2,3,3	0.88	0
3	EDO	C	804	-	3,3,3	0.09	0	2,2,2	0.25	0
5	BCT	D	803	-	3,3,3	0.92	0	2,3,3	1.63	1 (50%)

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	EDO	C	801	-	-	1/1/1/1	-
6	GOL	C	803	-	-	0/4/4/4	-
3	EDO	D	802	-	-	1/1/1/1	-
3	EDO	A	801	-	-	0/1/1/1	-
3	EDO	C	804	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	803	BCT	O2-C-O1	2.15	125.17	119.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	804	EDO	O1-C1-C2-O2
3	C	801	EDO	O1-C1-C2-O2
3	D	802	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	803	GOL	1	0
3	A	801	EDO	2	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	719/745 (96%)	0.26	20 (2%) 55 54	16, 42, 79, 138	1 (0%)
1	B	725/745 (97%)	0.42	25 (3%) 48 47	18, 49, 84, 119	1 (0%)
1	C	721/745 (96%)	0.31	25 (3%) 47 46	19, 46, 79, 150	2 (0%)
1	D	724/745 (97%)	0.17	21 (2%) 53 52	19, 40, 74, 118	3 (0%)
2	E	2/18 (11%)	2.26	2 (100%) 0 0	68, 68, 68, 71	0
2	F	2/18 (11%)	1.75	1 (50%) 0 1	65, 65, 65, 69	0
2	G	2/18 (11%)	1.76	1 (50%) 0 1	63, 63, 63, 76	0
2	H	2/18 (11%)	2.87	2 (100%) 0 0	70, 70, 70, 71	0
All	All	2897/3052 (94%)	0.29	97 (3%) 49 48	16, 44, 81, 150	7 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	664	TYR	5.4
1	D	664	TYR	4.3
1	B	664	TYR	4.3
1	A	664	TYR	4.1
1	B	663	ALA	4.1
1	B	456	LEU	3.9
1	B	230	GLY	3.7
1	C	143	GLY	3.5
1	A	697	LEU	3.5
1	A	444	TYR	3.5
1	B	662	ALA	3.4
1	A	141	LEU	3.4
1	B	700	GLY	3.3
1	D	699	SER	3.3
1	B	168	SER	3.3
1	A	245	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	731	THR	3.2
1	D	4	PRO	3.2
1	D	707	THR	3.2
2	H	804	VAL	3.2
1	B	704	GLY	3.2
1	A	168	SER	3.1
1	B	141	LEU	3.1
1	C	166	HIS	3.0
1	D	701	HIS	3.0
1	D	731	THR	3.0
1	C	700	GLY	3.0
1	D	663	ALA	2.9
1	D	697	LEU	2.9
1	D	167	GLY	2.8
1	D	710	MET	2.8
1	C	301	GLY	2.8
1	D	141	LEU	2.8
1	A	229	LYS	2.8
1	A	144	ASN	2.7
1	A	663	ALA	2.7
1	B	444	TYR	2.7
1	C	168	SER	2.6
1	C	704	GLY	2.6
1	C	701	HIS	2.6
1	C	663	ALA	2.6
2	H	807	SER	2.6
1	A	3	PHE	2.5
1	B	169	ASP	2.5
1	C	456	LEU	2.5
1	B	166	HIS	2.5
1	B	190	LYS	2.5
1	B	701	HIS	2.5
1	C	697	LEU	2.5
1	B	1	MET	2.5
2	E	807	SER	2.4
1	B	3	PHE	2.4
1	C	300	ILE	2.4
1	C	711	LEU	2.4
1	A	189	GLY	2.4
1	D	187	GLU	2.4
1	D	706	SER	2.4
1	C	206	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	804	VAL	2.4
1	C	707	THR	2.4
1	C	167	GLY	2.3
1	D	189	GLY	2.3
1	D	700	GLY	2.3
1	A	143	GLY	2.3
1	B	487	LEU	2.3
1	A	166	HIS	2.2
1	A	43	PHE	2.2
2	F	804	VAL	2.2
1	D	487	LEU	2.2
1	B	699	SER	2.2
1	A	184	PRO	2.2
1	C	115	ARG	2.2
1	C	126	SER	2.2
1	D	184	PRO	2.1
1	C	494	VAL	2.1
1	A	145	ALA	2.1
1	D	188	ARG	2.1
1	B	298	ASN	2.1
1	B	193	GLY	2.1
1	B	705	LYS	2.1
1	D	168	SER	2.1
1	B	224	GLU	2.1
1	B	731	THR	2.1
1	B	43	PHE	2.1
2	E	804	VAL	2.1
1	B	442	LYS	2.1
1	D	229	LYS	2.1
1	C	596	LEU	2.1
1	C	710	MET	2.1
1	D	165	GLU	2.1
1	A	652	THR	2.1
1	A	230	GLY	2.1
1	C	458	LEU	2.0
1	A	650	GLY	2.0
1	C	444[A]	TYR	2.0
1	C	662	ALA	2.0
1	C	4	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IML	G	802	9/10	0.60	0.28	76,87,114,122	0
2	IML	E	802	9/10	0.61	0.27	65,82,116,120	0
2	SAR	H	803	5/6	0.65	0.19	64,66,79,82	0
2	SAR	H	806	5/6	0.69	0.30	58,72,87,104	0
2	IML	F	802	9/10	0.71	0.27	73,98,131,145	0
2	MVA	E	808	8/9	0.72	0.25	63,85,97,98	0
2	SAR	E	806	5/6	0.76	0.22	53,57,72,74	0
2	MVA	F	808	8/9	0.80	0.18	63,82,91,91	0
2	MVA	H	808	8/9	0.80	0.20	56,83,90,108	0
2	SAR	G	806	5/6	0.81	0.20	49,70,79,93	0
2	SAR	G	803	5/6	0.82	0.17	79,83,88,106	0
2	MVA	G	808	8/9	0.82	0.17	50,73,91,92	0
2	SAR	E	803	5/6	0.82	0.18	67,68,77,81	0
2	SAR	F	803	5/6	0.84	0.19	66,80,88,98	0
2	SAR	F	806	5/6	0.84	0.22	61,69,82,90	0
2	IML	H	805	9/10	0.88	0.19	69,87,98,104	0
2	IML	F	805	9/10	0.89	0.16	58,68,82,91	0
2	IML	G	805	9/10	0.90	0.17	82,92,107,109	0
2	IML	E	805	9/10	0.90	0.17	62,74,84,100	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	A	806	1/1	0.56	0.31	70,70,70,70	0
4	NA	A	807	1/1	0.70	0.28	52,52,52,52	0
6	GOL	C	803	6/6	0.70	0.23	74,81,112,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BCT	D	803	4/4	0.71	0.14	61,64,86,94	0
4	NA	A	805	1/1	0.76	0.27	67,67,67,67	0
4	NA	B	804	1/1	0.81	0.17	61,61,61,61	0
4	NA	A	804	1/1	0.81	0.33	52,52,52,52	0
3	EDO	A	801	4/4	0.81	0.20	51,52,60,70	0
5	BCT	D	804	4/4	0.82	0.15	55,61,87,94	0
4	NA	B	803	1/1	0.82	0.21	50,50,50,50	0
4	NA	B	801	1/1	0.83	0.20	51,51,51,51	0
4	NA	D	806	1/1	0.83	0.18	47,47,47,47	0
5	BCT	C	802	4/4	0.83	0.14	51,68,72,89	0
3	EDO	C	804	4/4	0.84	0.33	47,60,61,62	0
4	NA	A	802	1/1	0.85	0.19	44,44,44,44	0
3	EDO	D	802	4/4	0.85	0.14	56,58,60,63	0
4	NA	C	807	1/1	0.85	0.27	53,53,53,53	0
4	NA	B	802	1/1	0.85	0.18	45,45,45,45	0
4	NA	A	803	1/1	0.86	0.33	48,48,48,48	0
4	NA	C	805	1/1	0.86	0.14	48,48,48,48	0
4	NA	C	806	1/1	0.88	0.15	48,48,48,48	0
3	EDO	C	801	4/4	0.88	0.13	43,44,46,55	0
5	BCT	D	801	4/4	0.88	0.10	43,51,52,67	0
4	NA	D	805	1/1	0.90	0.19	48,48,48,48	0
4	NA	D	807	1/1	0.93	0.16	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.