



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:45 PM UTC

PDB ID : 1XAE / pdb_00001xae
Title : Crystal structure of wild type yellow fluorescent protein zFP538 from *Zoanthus*
Authors : Remington, S.J.; Wachter, R.M.; Yarbrough, D.K.; Branchaud, B.; Anderson, D.C.; Kallio, K.; Lukyanov, K.A.
Deposited on : 2004-08-25
Resolution : 2.70 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

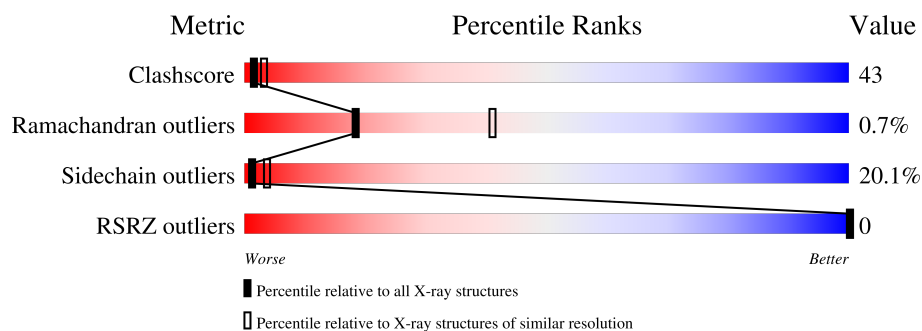
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	229	
1	B	229	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3616 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.

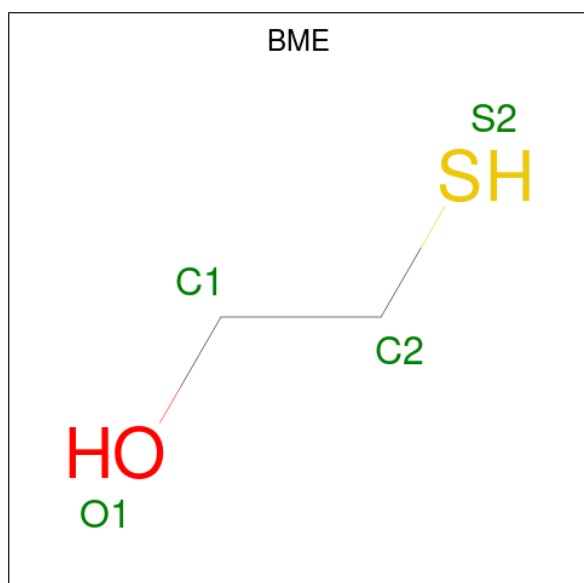
- Molecule 1 is a protein called fluorescent protein FP538.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1766	1135	293	321	17			
1	B	222	Total	C	N	O	S	0	0	0
			1759	1130	291	321	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CH7	LYS	chromophore	UNP 6090875
A	66	CH7	TYR	chromophore	UNP 6090875
A	66	CH7	GLY	chromophore	UNP 6090875
B	66	CH7	LYS	chromophore	UNP 6090875
B	66	CH7	TYR	chromophore	UNP 6090875
B	66	CH7	GLY	chromophore	UNP 6090875

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0

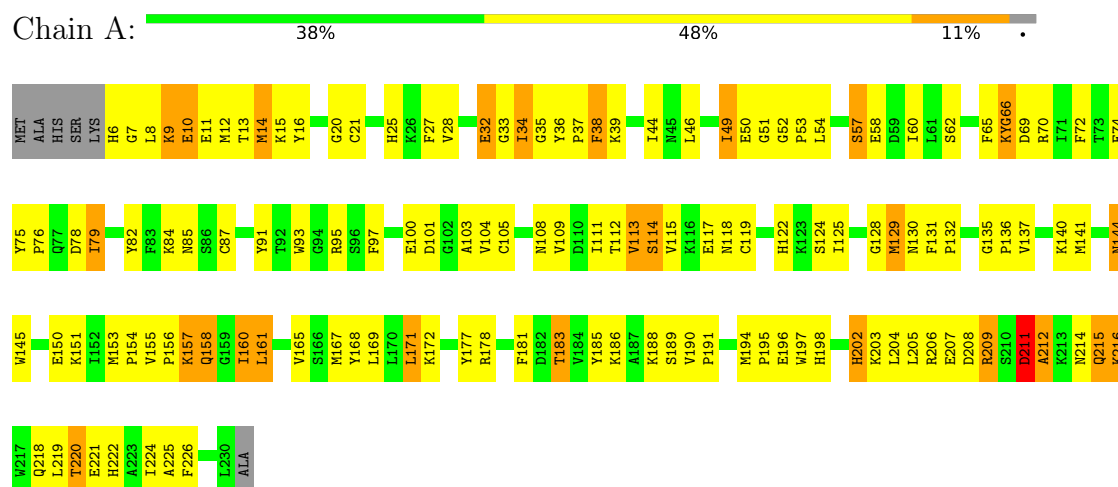
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total 43	O 43	0	0
3	B	40	Total 40	O 40	0	0

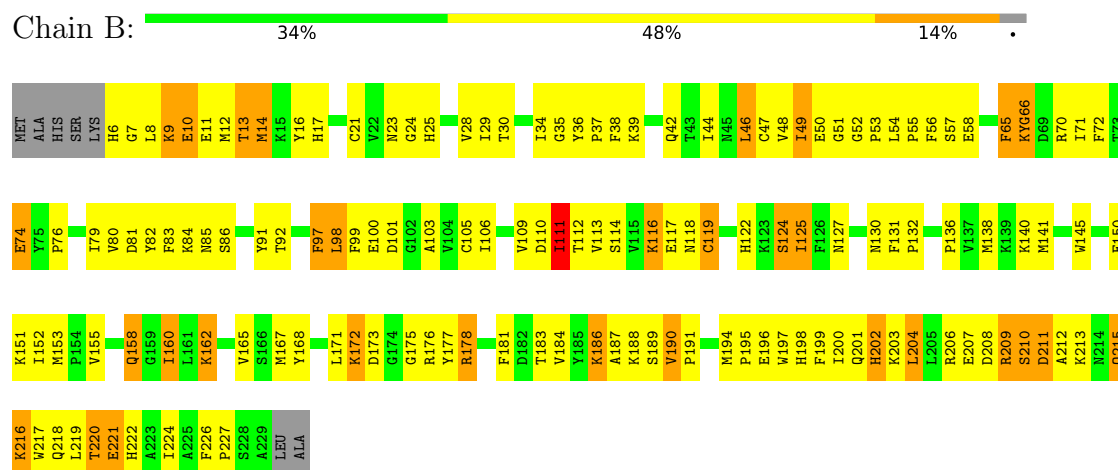
3 Residue-property plots

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: fluorescent protein FP538



• Molecule 1: fluorescent protein FP538



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.16Å 121.16Å 111.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (6.00-2.70) 90.3 (6.00-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.61Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.205 , 0.255 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3616	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BME, CSO, CH7, NFA

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	1.34	1/1761 (0.1%)	1.30	9/2375 (0.4%)
1	B	0.79	0/1754	1.29	10/2368 (0.4%)
All	All	1.10	1/3515 (0.0%)	1.29	19/4743 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	LYS	CB-CG	44.87	2.87	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	GLN	OE1-CD-NE2	-10.51	112.09	122.60
1	B	211	ASP	CA-CB-CG	10.34	122.94	112.60
1	A	215	GLN	OE1-CD-NE2	-10.22	112.38	122.60
1	A	113	VAL	N-CA-C	7.47	118.58	108.11
1	B	7	GLY	N-CA-C	-7.29	104.99	115.27
1	A	211	ASP	CA-CB-CG	7.25	119.85	112.60
1	A	215	GLN	CG-CD-NE2	7.00	126.91	116.40
1	B	215	GLN	CG-CD-NE2	6.96	126.83	116.40
1	A	212	ALA	N-CA-C	-6.45	104.61	114.16
1	B	38	PHE	CA-CB-CG	-6.12	107.68	113.80
1	B	178	ARG	N-CA-C	5.72	119.24	110.20
1	A	38	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	212	ALA	CA-C-O	5.46	124.53	118.52
1	B	113	VAL	N-CA-C	5.39	115.65	108.11
1	B	111	ILE	N-CA-C	5.36	115.82	107.99
1	A	7	GLY	N-CA-C	-5.24	107.88	115.27
1	B	181	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	213	LYS	N-CA-C	-5.12	107.59	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	N-CA-CB	5.04	119.00	110.49

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	1766	0	1687	146	0
1	B	1759	0	1672	150	0
2	A	4	0	5	1	0
2	B	4	0	5	0	0
3	A	43	0	0	4	0
3	B	40	0	0	6	0
All	All	3616	0	3369	295	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 43.

All (295) 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:B:76:PRO:HG2	1:B:79:ILE:HD12	1.18	1.16
1:A:28:VAL:HB	1:A:50:GLU:HB2	1.25	1.16
1:B:8:LEU:HD22	1:B:12:MET:HE1	1.35	1.07
1:B:141:MET:HE3	1:B:172:LYS:HG3	1.38	1.02
1:A:76:PRO:HG2	1:A:79:ILE:HG13	1.42	1.00
1:A:9:LYS:H	1:A:12:MET:HE2	1.26	0.97
1:A:62:SER:HB3	1:A:204:LEU:HD21	1.48	0.95
1:A:82:TYR:CE1	1:A:194:MET:HE1	2.02	0.94
1:B:82:TYR:CE1	1:B:194:MET:HE1	2.04	0.92
1:B:160:ILE:HG22	1:B:186:LYS:HB2	1.51	0.91
1:A:28:VAL:HG12	1:A:49:ILE:HG12	1.51	0.91
1:A:97:PHE:HB2	1:A:105:CYS:HB2	1.54	0.89
1:B:209:ARG:HG2	1:B:209:ARG:HH11	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:HG22	1:B:124:SER:HB3	1.55	0.88
1:A:28:VAL:HB	1:A:50:GLU:CB	2.05	0.86
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.40	0.86
1:B:82:TYR:HE1	1:B:194:MET:HE1	1.41	0.86
1:B:150:GLU:HB2	1:B:165:VAL:HB	1.58	0.85
1:B:28:VAL:HB	1:B:50:GLU:HB2	1.59	0.83
1:A:6:HIS:HB3	1:A:87:CYS:HB2	1.60	0.82
1:A:76:PRO:HG2	1:A:79:ILE:CG1	2.08	0.82
1:B:14:MET:HE1	1:B:35:GLY:HA3	1.60	0.81
1:B:160:ILE:CG2	1:B:186:LYS:HB2	2.10	0.81
1:A:82:TYR:HE1	1:A:194:MET:HE1	1.44	0.81
1:A:111:ILE:HD12	1:A:122:HIS:HD2	1.46	0.81
1:B:111:ILE:HD13	1:B:122:HIS:HD2	1.44	0.80
1:B:23:ASN:HD21	1:B:131:PHE:HB2	1.47	0.79
1:A:66:CH7:NZ	1:A:66:CH7:HA31	1.96	0.79
1:A:112:THR:HG22	1:A:188:LYS:HZ3	1.46	0.79
1:B:111:ILE:HD13	1:B:122:HIS:CD2	2.18	0.78
1:B:209:ARG:HG2	1:B:209:ARG:NH1	1.96	0.78
1:B:76:PRO:CG	1:B:79:ILE:HD12	2.06	0.77
1:A:9:LYS:H	1:A:12:MET:CE	1.98	0.77
1:A:8:LEU:CD1	1:A:84:LYS:HG2	2.15	0.77
1:B:14:MET:HE1	1:B:35:GLY:CA	2.15	0.76
1:A:9:LYS:N	1:A:12:MET:HE2	2.01	0.76
1:B:13:THR:HG22	1:B:34:ILE:HD13	1.67	0.76
1:A:209:ARG:HG2	1:A:209:ARG:NH1	1.97	0.76
1:A:112:THR:HG22	1:A:188:LYS:NZ	1.99	0.75
1:B:23:ASN:ND2	1:B:131:PHE:HB2	2.01	0.75
1:B:12:MET:HE3	1:B:37:PRO:HG3	1.68	0.75
1:B:9:LYS:HG3	1:B:118:ASN:OD1	1.86	0.75
1:A:8:LEU:HD23	1:A:12:MET:HE3	1.69	0.74
1:B:98:LEU:HD22	3:B:590:HOH:O	1.87	0.74
1:B:8:LEU:CD2	1:B:12:MET:HE1	2.16	0.74
1:A:14:MET:HE1	1:A:35:GLY:HA3	1.70	0.73
1:A:154:PRO:HG3	1:A:195:PRO:O	1.89	0.72
1:A:145:TRP:CZ3	1:A:167:MET:HB3	2.24	0.72
1:B:92:THR:HG22	1:B:110:ASP:HA	1.71	0.72
1:A:109:VAL:HG22	1:A:124:SER:HB3	1.72	0.72
1:B:66:CH7:HG1	1:B:221:GLU:HB2	1.71	0.71
1:A:191:PRO:HG2	1:A:194:MET:HE3	1.73	0.71
1:B:66:CH7:NZ	1:B:66:CH7:HA31	2.04	0.71
1:A:160:ILE:HG22	1:A:186:LYS:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PRO:HG2	1:B:79:ILE:CD1	2.11	0.70
1:A:141:MET:HE3	1:A:172:LYS:HG3	1.73	0.70
1:A:151:LYS:HE3	1:A:197:TRP:CE3	2.26	0.69
1:A:111:ILE:HD12	1:A:122:HIS:CD2	2.28	0.69
1:A:11:GLU:HG3	1:A:36:TYR:CZ	2.27	0.69
1:B:150:GLU:HB3	1:B:202:HIS:HE1	1.56	0.69
1:B:100:GLU:HG2	1:B:177:TYR:CE1	2.27	0.69
1:B:207:GLU:HG2	1:B:209:ARG:CD	2.24	0.68
1:A:11:GLU:HG3	1:A:36:TYR:CE2	2.29	0.67
1:B:130:ASN:O	1:B:132:PRO:HD3	1.95	0.66
1:B:202:HIS:HB3	1:B:221:GLU:OE2	1.95	0.66
1:B:168:TYR:CE2	1:B:178:ARG:HG3	2.31	0.65
1:A:130:ASN:O	1:A:132:PRO:HD3	1.96	0.65
1:B:11:GLU:HG3	1:B:36:TYR:CE2	2.31	0.65
1:A:28:VAL:CG1	1:A:49:ILE:HG12	2.27	0.65
1:A:207:GLU:CD	1:A:209:ARG:HE	2.05	0.65
1:B:13:THR:CG2	1:B:34:ILE:HD13	2.26	0.65
1:B:66:CH7:HD1	1:B:66:CH7:N2	2.10	0.65
1:B:191:PRO:CG	1:B:194:MET:HE3	2.27	0.65
1:A:113:VAL:HG11	2:A:587:BME:H12	1.79	0.64
1:B:101:ASP:OD1	1:B:132:PRO:HG2	1.97	0.64
1:B:209:ARG:O	1:B:216:LYS:NZ	2.30	0.64
1:A:6:HIS:CE1	1:A:85:ASN:HA	2.32	0.64
1:A:82:TYR:CD1	1:A:194:MET:HE1	2.32	0.64
1:A:54:LEU:O	1:A:140:LYS:NZ	2.30	0.64
1:A:58:GLU:OE1	1:A:206:ARG:HD2	1.97	0.63
1:B:191:PRO:HG2	1:B:194:MET:HE3	1.79	0.63
1:A:21:CSO:HA	1:A:25:HIS:O	1.99	0.63
1:A:10:GLU:O	1:A:37:PRO:HD2	1.99	0.63
1:A:191:PRO:CG	1:A:194:MET:HE3	2.29	0.63
1:B:54:LEU:O	1:B:140:LYS:NZ	2.32	0.63
1:A:8:LEU:HD13	1:A:84:LYS:HG2	1.82	0.61
1:A:14:MET:HE1	1:A:35:GLY:CA	2.31	0.61
1:A:158:GLN:HB3	1:A:160:ILE:HG13	1.81	0.61
1:B:14:MET:HE1	1:B:35:GLY:N	2.15	0.61
1:A:8:LEU:HD11	1:A:84:LYS:HG2	1.82	0.61
1:B:208:ASP:O	1:B:209:ARG:HD2	2.00	0.61
1:A:66:CH7:N2	1:A:66:CH7:HD1	2.13	0.61
1:A:35:GLY:HA3	1:A:72:PHE:CE2	2.36	0.60
1:A:70:ARG:HA	1:A:70:ARG:NE	2.16	0.60
1:A:8:LEU:HA	1:A:12:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HB2	1:B:221:GLU:HG3	1.83	0.60
1:B:11:GLU:HB2	1:B:36:TYR:HE2	1.64	0.60
1:B:209:ARG:HH11	1:B:209:ARG:CG	2.13	0.60
1:B:210:SER:HB3	1:B:215:GLN:HA	1.83	0.60
1:A:101:ASP:OD1	1:A:132:PRO:HG2	2.01	0.60
1:A:111:ILE:CD1	1:A:122:HIS:HD2	2.14	0.60
1:B:186:LYS:HG2	3:B:618:HOH:O	2.01	0.59
1:A:207:GLU:O	1:A:209:ARG:HD2	2.02	0.59
1:A:140:LYS:O	1:A:172:LYS:NZ	2.30	0.59
1:A:155:VAL:HG12	1:A:158:GLN:HB2	1.84	0.59
1:B:141:MET:HA	1:B:172:LYS:HE3	1.85	0.58
1:A:191:PRO:HB2	1:A:194:MET:HE3	1.85	0.58
1:B:46:LEU:HD11	1:B:219:LEU:HD12	1.85	0.58
1:B:42:GLN:HE22	1:B:72:PHE:HB2	1.68	0.58
1:B:10:GLU:O	1:B:37:PRO:HD2	2.03	0.58
1:B:6:HIS:HE1	1:B:85:ASN:ND2	2.01	0.57
1:A:150:GLU:HB2	1:A:165:VAL:HB	1.86	0.57
1:B:11:GLU:HB2	1:B:36:TYR:CE2	2.39	0.57
1:A:160:ILE:CG2	1:A:186:LYS:HG3	2.35	0.57
1:B:145:TRP:CZ3	1:B:167:MET:HB3	2.39	0.57
1:B:46:LEU:HD13	1:B:217:TRP:NE1	2.20	0.57
1:B:141:MET:O	1:B:172:LYS:HG2	2.05	0.56
1:A:168:TYR:CZ	1:A:178:ARG:HD2	2.40	0.56
1:A:208:ASP:O	1:A:209:ARG:HD2	2.05	0.56
1:A:191:PRO:CB	1:A:194:MET:HE3	2.36	0.56
1:B:13:THR:O	1:B:119:CYS:HA	2.05	0.56
1:B:80:VAL:HB	1:B:195:PRO:HB3	1.87	0.56
1:A:14:MET:HB2	1:A:122:HIS:HE1	1.71	0.56
1:B:9:LYS:O	1:B:37:PRO:HG2	2.06	0.56
1:A:150:GLU:HB3	1:A:202:HIS:HE1	1.71	0.56
1:B:82:TYR:CD1	1:B:194:MET:HE1	2.41	0.56
1:B:136:PRO:HB3	1:B:171:LEU:HD22	1.89	0.55
1:A:76:PRO:HG2	1:A:79:ILE:CD1	2.37	0.55
1:A:11:GLU:HB2	1:A:36:TYR:HE2	1.71	0.55
1:A:36:TYR:HB2	1:A:39:LYS:HB2	1.89	0.55
1:A:82:TYR:CG	1:A:161:LEU:HD22	2.42	0.55
1:A:214:ASN:HB3	1:A:216:LYS:HD3	1.88	0.54
1:B:151:LYS:HE3	1:B:197:TRP:CE3	2.42	0.54
1:B:81:ASP:OD2	1:B:84:LYS:HG3	2.07	0.54
1:A:9:LYS:O	1:A:37:PRO:HG2	2.08	0.54
1:B:53:PRO:HA	1:B:215:GLN:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PRO:O	1:A:157:LYS:HB2	2.08	0.54
1:B:162:LYS:HE2	3:B:592:HOH:O	2.07	0.54
1:B:222:HIS:CE1	1:B:224:ILE:HD11	2.43	0.54
1:A:155:VAL:CG2	1:A:160:ILE:HD12	2.38	0.53
1:B:28:VAL:HG11	1:B:49:ILE:HD11	1.90	0.53
1:A:136:PRO:HB3	1:A:171:LEU:HD22	1.89	0.53
1:B:12:MET:CE	1:B:37:PRO:HG3	2.36	0.53
1:A:82:TYR:CD2	1:A:161:LEU:HD22	2.43	0.53
1:B:28:VAL:HG12	1:B:49:ILE:HG13	1.91	0.53
1:B:70:ARG:NE	1:B:70:ARG:HA	2.24	0.53
1:B:111:ILE:CD1	1:B:122:HIS:HD2	2.18	0.53
1:B:155:VAL:HG21	1:B:160:ILE:HD12	1.91	0.53
1:A:93:TRP:CZ2	1:A:109:VAL:HG21	2.42	0.53
1:A:11:GLU:HB2	1:A:36:TYR:CE2	2.44	0.52
1:A:136:PRO:O	1:A:141:MET:N	2.36	0.52
1:B:202:HIS:ND1	1:B:202:HIS:N	2.58	0.52
1:A:157:LYS:CB	1:A:157:LYS:CG	2.87	0.52
1:A:155:VAL:HG21	1:A:160:ILE:CD1	2.40	0.52
1:B:35:GLY:HA3	1:B:72:PHE:CE2	2.45	0.52
1:B:158:GLN:HB3	1:B:160:ILE:HG13	1.90	0.52
1:A:15:LYS:NZ	1:A:32:GLU:HB3	2.24	0.52
1:A:8:LEU:HD23	1:A:12:MET:CE	2.38	0.52
1:A:6:HIS:HB3	1:A:87:CYS:CB	2.35	0.52
1:A:198:HIS:HB2	1:A:226:PHE:O	2.10	0.52
1:B:28:VAL:CG1	1:B:49:ILE:HD11	2.40	0.52
1:A:136:PRO:HA	1:A:141:MET:HB2	1.92	0.51
1:A:221:GLU:HG2	1:A:222:HIS:N	2.25	0.51
1:B:21:CSO:SG	1:B:24:GLY:HA2	2.50	0.51
1:A:25:HIS:NE2	1:A:51:GLY:O	2.36	0.51
1:A:207:GLU:OE2	1:A:209:ARG:NE	2.43	0.51
1:A:136:PRO:CB	1:A:171:LEU:HD22	2.41	0.50
1:A:196:GLU:O	1:A:197:TRP:C	2.55	0.50
1:B:23:ASN:HD21	1:B:131:PHE:CB	2.22	0.50
1:B:91:TYR:N	1:B:188:LYS:HD2	2.25	0.50
1:B:222:HIS:HE1	3:B:627:HOH:O	1.95	0.50
1:B:222:HIS:NE2	1:B:224:ILE:HD11	2.26	0.50
1:B:150:GLU:HB3	1:B:202:HIS:CE1	2.42	0.50
1:A:36:TYR:CB	1:A:39:LYS:HB2	2.42	0.50
1:A:155:VAL:HG21	1:A:160:ILE:HD12	1.94	0.50
1:B:74:GLU:HG2	1:B:224:ILE:HG23	1.93	0.50
1:A:70:ARG:HA	1:A:70:ARG:CZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:SER:HB3	1:A:117:GLU:HB2	1.94	0.50
1:B:97:PHE:HB2	1:B:105:CYS:HB2	1.94	0.50
1:B:6:HIS:CE1	1:B:85:ASN:ND2	2.79	0.49
1:B:207:GLU:OE2	1:B:209:ARG:NE	2.28	0.49
1:A:57:SER:HB3	1:A:137:VAL:HA	1.93	0.49
1:B:99:PHE:HB3	1:B:177:TYR:OH	2.12	0.49
1:B:55:PRO:HD2	1:B:56:PHE:CE2	2.47	0.49
1:A:52:GLY:HA2	1:A:53:PRO:C	2.36	0.49
1:A:14:MET:HB2	1:A:122:HIS:CE1	2.47	0.49
1:A:13:THR:O	1:A:119:CYS:HA	2.12	0.49
1:B:198:HIS:HB2	1:B:226:PHE:O	2.14	0.48
1:A:38:PHE:HB2	3:A:592:HOH:O	2.13	0.48
1:B:116:LYS:HG3	1:B:117:GLU:HG2	1.94	0.48
1:A:114:SER:O	1:A:118:ASN:N	2.47	0.48
1:A:220:THR:HG22	1:A:220:THR:O	2.13	0.48
1:B:100:GLU:HG2	1:B:177:TYR:CD1	2.49	0.48
1:A:8:LEU:HA	1:A:12:MET:HE1	1.95	0.47
1:B:29:ILE:HD13	1:B:217:TRP:HH2	1.79	0.47
1:B:42:GLN:NE2	1:B:72:PHE:HB2	2.29	0.47
1:B:125:ILE:O	1:B:125:ILE:HG22	2.15	0.47
1:A:209:ARG:HH11	1:A:209:ARG:CG	2.16	0.47
1:A:75:TYR:HA	1:A:225:ALA:HB3	1.97	0.46
1:A:103:ALA:HB2	1:A:131:PHE:HA	1.97	0.46
1:A:12:MET:O	1:A:34:ILE:HA	2.15	0.46
1:A:11:GLU:CB	1:A:36:TYR:CE2	2.99	0.46
1:A:104:VAL:HG12	1:B:106:ILE:HD11	1.97	0.46
1:A:168:TYR:CE2	1:A:178:ARG:HD2	2.50	0.46
1:B:17:HIS:HD2	1:B:30:THR:HG22	1.80	0.46
1:A:171:LEU:HD21	1:A:177:TYR:HB2	1.98	0.46
1:A:93:TRP:CZ2	1:A:109:VAL:CG2	2.99	0.46
1:A:144:ASN:OD1	1:A:205:LEU:HA	2.16	0.46
1:B:9:LYS:H	1:B:12:MET:HE2	1.80	0.46
1:B:204:LEU:HB2	1:B:221:GLU:CG	2.46	0.46
1:A:95:ARG:HB2	1:A:183:THR:HG23	1.96	0.46
1:B:11:GLU:CB	1:B:36:TYR:CE2	2.99	0.46
1:B:28:VAL:HG12	1:B:49:ILE:CG1	2.46	0.45
1:A:135:GLY:HA3	3:A:596:HOH:O	2.16	0.45
1:B:11:GLU:CG	1:B:36:TYR:CE2	2.99	0.45
1:B:191:PRO:CB	1:B:194:MET:HE3	2.46	0.45
1:A:53:PRO:HA	1:A:215:GLN:OE1	2.16	0.45
1:A:109:VAL:HG22	1:A:124:SER:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LYS:O	1:A:221:GLU:HA	2.16	0.45
1:A:14:MET:HE1	1:A:35:GLY:N	2.32	0.45
1:B:49:ILE:O	1:B:50:GLU:HG3	2.17	0.44
1:A:6:HIS:N	3:A:614:HOH:O	2.50	0.44
1:A:11:GLU:CG	1:A:36:TYR:CE2	2.99	0.44
1:A:103:ALA:CB	1:A:131:PHE:CD2	3.00	0.44
1:A:129:MET:HE2	1:A:129:MET:HB2	1.85	0.44
1:A:9:LYS:HB2	1:A:12:MET:SD	2.58	0.44
1:A:145:TRP:CE3	1:A:167:MET:HB3	2.52	0.44
1:B:97:PHE:CD1	1:B:97:PHE:N	2.86	0.44
1:B:47:CSO:O	1:B:49:ILE:HG23	2.18	0.44
1:A:35:GLY:HA3	1:A:72:PHE:HE2	1.82	0.44
1:A:91:TYR:N	1:A:188:LYS:HD2	2.33	0.43
1:A:222:HIS:CE1	1:A:224:ILE:HD11	2.53	0.43
1:B:158:GLN:HB3	1:B:160:ILE:CG1	2.48	0.43
1:B:70:ARG:HB2	1:B:83:PHE:CD2	2.53	0.43
1:B:91:TYR:CB	1:B:187:ALA:HA	2.48	0.43
1:A:8:LEU:HA	1:A:12:MET:HE2	2.01	0.43
1:A:211:ASP:HB2	1:A:212:ALA:H	1.28	0.43
1:B:100:GLU:CG	1:B:177:TYR:CE1	2.99	0.43
1:B:14:MET:HB2	1:B:122:HIS:CE1	2.52	0.43
1:B:56:PHE:CD2	1:B:56:PHE:N	2.87	0.43
1:B:8:LEU:HD12	1:B:84:LYS:HD3	2.00	0.43
1:A:13:THR:HA	1:A:33:GLY:O	2.19	0.43
1:A:101:ASP:CG	1:A:132:PRO:HG2	2.44	0.43
1:B:91:TYR:HB2	1:B:187:ALA:HA	2.00	0.43
1:B:116:LYS:CG	1:B:117:GLU:HG2	2.49	0.43
1:B:101:ASP:CG	1:B:132:PRO:HG2	2.44	0.43
1:B:25:HIS:NE2	1:B:51:GLY:O	2.52	0.42
1:B:197:TRP:CZ3	1:B:199:PHE:CZ	3.07	0.42
1:A:46:LEU:HD11	1:A:219:LEU:HD12	2.01	0.42
1:A:161:LEU:HB2	1:A:185:TYR:HB2	2.01	0.42
1:A:165:VAL:HG12	1:A:181:PHE:HB2	2.01	0.42
1:B:42:GLN:O	1:B:220:THR:HA	2.19	0.42
1:B:98:LEU:HD12	1:B:98:LEU:HA	1.78	0.42
1:A:14:MET:HG3	1:A:16:TYR:OH	2.20	0.42
1:A:20:GLY:HA3	1:A:27:PHE:CZ	2.55	0.42
1:A:57:SER:O	1:A:60:ILE:HG12	2.20	0.42
1:A:145:TRP:CZ3	1:A:167:MET:CB	3.00	0.42
1:B:11:GLU:HG2	1:B:12:MET:N	2.34	0.42
1:B:65:NFA:O	1:B:66:CH7:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:HG22	1:B:184:VAL:N	2.35	0.42
1:A:165:VAL:CG1	1:A:181:PHE:HB2	2.50	0.42
1:B:48:VAL:HG23	1:B:217:TRP:HZ3	1.85	0.42
1:B:55:PRO:HD2	1:B:56:PHE:CD2	2.55	0.42
1:B:189:SER:HB2	3:B:608:HOH:O	2.19	0.42
1:B:206:ARG:HB2	1:B:219:LEU:CD2	2.50	0.42
1:B:162:LYS:HE2	1:B:162:LYS:HB3	1.71	0.42
1:B:127:ASN:ND2	3:B:598:HOH:O	2.29	0.41
1:B:14:MET:HB2	1:B:122:HIS:HE1	1.84	0.41
1:B:52:GLY:HA2	1:B:53:PRO:C	2.43	0.41
1:B:155:VAL:CG2	1:B:162:LYS:CG	2.98	0.41
1:B:29:ILE:HD13	1:B:217:TRP:CH2	2.54	0.41
1:B:114:SER:O	1:B:118:ASN:N	2.53	0.41
1:B:80:VAL:HB	1:B:195:PRO:CB	2.50	0.41
1:B:190:VAL:HA	1:B:191:PRO:HD3	1.91	0.41
1:A:9:LYS:HA	1:A:9:LYS:HD2	1.80	0.41
1:A:69:ASP:HB2	3:A:595:HOH:O	2.20	0.41
1:A:104:VAL:O	1:A:128:GLY:HA2	2.20	0.41
1:B:171:LEU:HG	1:B:175:GLY:O	2.19	0.41
1:B:70:ARG:CB	1:B:83:PHE:CD2	3.04	0.41
1:A:74:GLU:O	1:A:74:GLU:HG2	2.18	0.41
1:A:82:TYR:CG	1:A:161:LEU:CD2	3.04	0.41
1:B:103:ALA:CB	1:B:131:PHE:CD2	3.04	0.41
1:B:145:TRP:CE3	1:B:167:MET:HB3	2.56	0.41
1:A:167:MET:HG3	1:A:181:PHE:CZ	2.56	0.41
1:B:66:CH7:CG	1:B:221:GLU:HB2	2.45	0.41
1:B:191:PRO:CB	1:B:194:MET:CE	2.99	0.40
1:B:152:ILE:HG13	1:B:200:ILE:HG13	2.03	0.40
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.92	0.40
1:B:8:LEU:HB3	1:B:12:MET:CE	2.51	0.40
1:B:16:TYR:O	1:B:30:THR:HA	2.21	0.40
1:B:105:CYS:HA	1:B:127:ASN:O	2.22	0.40
1:B:207:GLU:HG2	1:B:209:ARG:HD2	2.00	0.40
1:A:112:THR:CG2	1:A:188:LYS:NZ	2.80	0.40
1:B:36:TYR:HB2	1:B:39:LYS:HB2	2.03	0.40
1:B:100:GLU:HG2	1:B:177:TYR:HE1	1.83	0.40

There are no symmetry-related clashes.

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	216/229 (94%)	204 (94%)	11 (5%)	1 (0%)	24	48
1	B	215/229 (94%)	207 (96%)	6 (3%)	2 (1%)	14	35
All	All	431/458 (94%)	411 (95%)	17 (4%)	3 (1%)	18	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	VAL
1	B	212	ALA
1	B	227	PRO

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	182/194 (94%)	151 (83%)	31 (17%)	2	6
1	B	181/194 (93%)	139 (77%)	42 (23%)	1	2
All	All	363/388 (94%)	290 (80%)	73 (20%)	1	4

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	10	GLU
1	A	14	MET

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Mol	Chain	Res	Type
1	A	32	GLU
1	A	34	ILE
1	A	44	ILE
1	A	49	ILE
1	A	57	SER
1	A	78	ASP
1	A	79	ILE
1	A	100	GLU
1	A	108	ASN
1	A	114	SER
1	A	125	ILE
1	A	129	MET
1	A	144	ASN
1	A	153	MET
1	A	158	GLN
1	A	160	ILE
1	A	161	LEU
1	A	169	LEU
1	A	171	LEU
1	A	183	THR
1	A	189	SER
1	A	190	VAL
1	A	202	HIS
1	A	209	ARG
1	A	211	ASP
1	A	216	LYS
1	A	218	GLN
1	A	220	THR
1	B	9	LYS
1	B	10	GLU
1	B	13	THR
1	B	14	MET
1	B	44	ILE
1	B	46	LEU
1	B	49	ILE
1	B	57	SER
1	B	58	GLU
1	B	71	ILE
1	B	74	GLU
1	B	86	SER
1	B	97	PHE
1	B	98	LEU

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Mol	Chain	Res	Type
1	B	111	ILE
1	B	112	THR
1	B	116	LYS
1	B	119	CYS
1	B	124	SER
1	B	125	ILE
1	B	138	MET
1	B	153	MET
1	B	158	GLN
1	B	160	ILE
1	B	162	LYS
1	B	172	LYS
1	B	173	ASP
1	B	176	ARG
1	B	186	LYS
1	B	190	VAL
1	B	196	GLU
1	B	201	GLN
1	B	202	HIS
1	B	203	LYS
1	B	204	LEU
1	B	209	ARG
1	B	210	SER
1	B	211	ASP
1	B	216	LYS
1	B	218	GLN
1	B	220	THR
1	B	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	45	ASN
1	A	118	ASN
1	A	158	GLN
1	A	180	GLN
1	A	202	HIS
1	B	6	HIS
1	B	17	HIS
1	B	42	GLN
1	B	85	ASN

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Mol	Chain	Res	Type
1	B	180	GLN
1	B	201	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
1	CSO	A	21	1	3,6,7	0.81	0	1,6,8	0.37	0
1	CSO	B	21	1	3,6,7	0.96	0	1,6,8	0.38	0
1	NFA	B	65	1	12,12,12	1.60	2 (16%)	15,15,15	0.73	0
1	CH7	B	66	1	24,25,26	2.44	11 (45%)	28,34,36	1.38	5 (17%)
1	CSO	B	47	1	3,6,7	0.97	0	1,6,8	0.03	0
1	NFA	A	65	1	12,12,12	1.42	2 (16%)	15,15,15	0.92	1 (6%)
1	CSO	A	47	1	3,6,7	0.86	0	1,6,8	0.38	0
1	CH7	A	66	1	24,25,26	2.44	12 (50%)	28,34,36	1.43	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	21	1	-	0/1/5/7	-
1	CSO	B	21	1	-	0/1/5/7	-
1	NFA	B	65	1	-	5/8/8/8	0/1/1/1
1	CH7	B	66	1	-	1/6/35/36	0/3/3/3
1	CSO	B	47	1	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NFA	A	65	1	-	5/8/8/8	0/1/1/1
1	CSO	A	47	1	-	0/1/5/7	-
1	CH7	A	66	1	-	1/6/35/36	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CH7	OH-CZ	-5.09	1.25	1.37
1	A	66	CH7	OH-CZ	-5.01	1.25	1.37
1	A	66	CH7	CG2-CB2	-4.04	1.39	1.46
1	B	66	CH7	CG2-CB2	-4.04	1.39	1.46
1	B	66	CH7	CE1-CZ	4.04	1.46	1.39
1	A	66	CH7	CE1-CZ	4.02	1.46	1.39
1	B	65	NFA	O-C	4.02	1.31	1.23
1	A	66	CH7	CE2-CZ	3.82	1.46	1.39
1	A	65	NFA	O-C	3.69	1.30	1.23
1	B	66	CH7	CE2-CZ	3.56	1.45	1.39
1	B	66	CH7	C1-N3	3.44	1.43	1.38
1	B	65	NFA	C-NXT	3.35	1.40	1.32
1	A	66	CH7	C1-N3	3.33	1.43	1.38
1	A	66	CH7	CB2-CA2	3.31	1.38	1.35
1	B	66	CH7	CB-CA1	3.28	1.55	1.50
1	A	66	CH7	CB-CA1	3.13	1.55	1.50
1	B	66	CH7	CB2-CA2	3.07	1.38	1.35
1	B	66	CH7	CA3-N3	-2.93	1.41	1.47
1	A	65	NFA	C-NXT	2.82	1.39	1.32
1	A	66	CH7	CA3-N3	-2.40	1.42	1.47
1	B	66	CH7	C1-CA1	2.28	1.51	1.48
1	A	66	CH7	C1-CA1	2.27	1.51	1.48
1	A	66	CH7	CE-NZ	-2.24	1.42	1.47
1	B	66	CH7	CD1-CG2	2.22	1.44	1.39
1	A	66	CH7	CD2-CG2	2.14	1.43	1.39
1	A	66	CH7	CD1-CG2	2.09	1.43	1.39
1	B	66	CH7	CD2-CG2	2.02	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CH7	CE1-CZ-CE2	-3.15	114.76	119.77
1	A	66	CH7	CE1-CZ-CE2	-3.15	114.76	119.77
1	A	66	CH7	C3-CA3-N3	2.79	118.77	112.43
1	A	66	CH7	CE-NZ-CA1	-2.67	112.41	117.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CH7	CE-NZ-CA1	-2.59	112.56	117.44
1	A	66	CH7	CD2-CE2-CZ	2.38	122.40	119.88
1	B	66	CH7	C3-CA3-N3	2.38	117.83	112.43
1	B	66	CH7	CD2-CE2-CZ	2.19	122.20	119.88
1	A	65	NFA	C-CA-N	2.18	117.53	109.43
1	B	66	CH7	O2-C2-CA2	2.11	132.37	131.02

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	NFA	NXT-C-CA-N
1	A	65	NFA	O-C-CA-CB
1	B	65	NFA	NXT-C-CA-N
1	A	66	CH7	C3-CA3-N3-C2
1	B	66	CH7	C3-CA3-N3-C2
1	A	65	NFA	NXT-C-CA-CB
1	B	65	NFA	O-C-CA-N
1	A	65	NFA	C-CA-CB-CG
1	A	65	NFA	O-C-CA-N
1	B	65	NFA	O-C-CA-CB
1	B	65	NFA	C-CA-CB-CG
1	B	65	NFA	NXT-C-CA-CB

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	21	CSO	1	0
1	B	21	CSO	1	0
1	B	65	NFA	1	0
1	B	66	CH7	5	0
1	B	47	CSO	1	0
1	A	66	CH7	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BME	B	587	1	3,3,3	0.92	0	2,2,2	1.12	0
2	BME	A	587	1	3,3,3	0.56	0	2,2,2	0.66	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
2	BME	B	587	1	-	1/1/1/1	-
2	BME	A	587	1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	587	BME	O1-C1-C2-S2
2	B	587	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	587	BME	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	219/229 (95%)	-0.98	0 100 100	38, 52, 75, 91	0
1	B	218/229 (95%)	-0.97	0 100 100	33, 54, 74, 97	0
All	All	437/458 (95%)	-0.97	0 100 100	33, 53, 74, 97	0

There are no RSRZ outliers to report.

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
1	CSO	B	21	7/8	0.93	0.07	49,56,62,70	0
1	CSO	A	21	7/8	0.95	0.05	34,50,56,64	0
1	CH7	B	66	23/24	0.95	0.05	29,57,100,100	0
1	CSO	B	47	7/8	0.97	0.05	48,50,73,96	0
1	NFA	B	65	12/12	0.97	0.04	43,48,61,100	0
1	CH7	A	66	23/24	0.97	0.05	42,62,100,100	0
1	NFA	A	65	12/12	0.98	0.05	34,47,66,69	0
1	CSO	A	47	7/8	0.98	0.04	40,49,81,94	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(\AA^2)	Q<0.9
2	BME	A	587	4/4	0.95	0.07	39,82,97,100	0
2	BME	B	587	4/4	0.97	0.06	54,67,73,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.