



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:07 PM UTC

PDB ID : 2ZSU / pdb_00002zsu
Title : Crystal structure of spermidine synthase from *Pyrococcus horikoshii* OT3, P1 form
Authors : Mizutani, H.; Kunishima, N.
Deposited on : 2008-09-17
Resolution : 2.20 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:

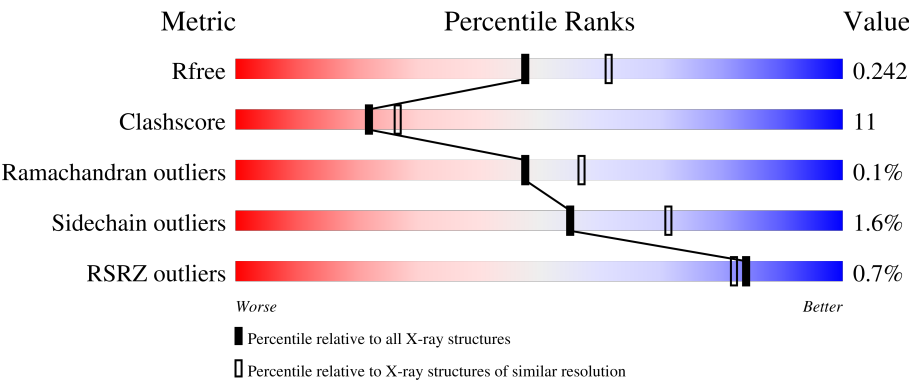
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	280	% 76%22%.
1	B	280	% 75%23%..
1	C	280	73%24%..
1	D	280	75%21%..
1	E	280	79%20%.

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Mol	Chain	Length	Quality of chain
1	F	280	% 71% 26% ..

2 Entry composition [i](#)

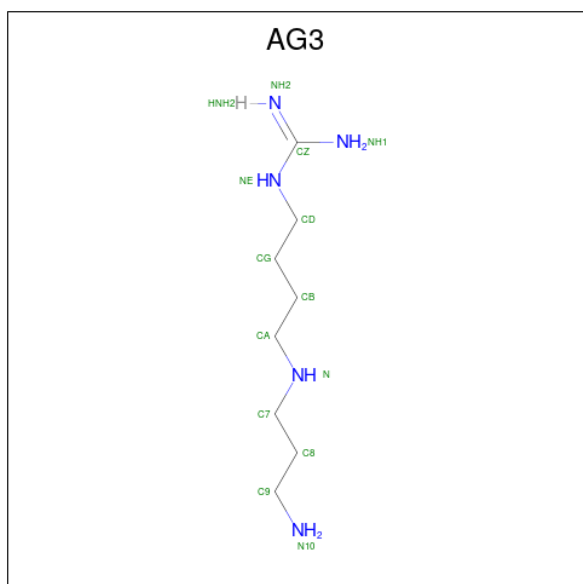
There are 3 unique types of molecules in this entry. The entry contains 14310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2256	1467	359	420	10			
1	B	278	Total	C	N	O	S	0	0	0
			2237	1456	354	418	9			
1	C	273	Total	C	N	O	S	0	0	0
			2204	1437	349	409	9			
1	D	271	Total	C	N	O	S	0	0	0
			2190	1427	347	407	9			
1	E	279	Total	C	N	O	S	0	0	0
			2248	1462	358	419	9			
1	F	273	Total	C	N	O	S	0	0	0
			2206	1437	349	411	9			

- Molecule 2 is 1-{4-[(3-aminopropyl)amino]butyl}guanidine (CCD ID: AG3) (formula: $C_8H_{21}N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 13 8 5	0	0
2	C	1	Total C N 13 8 5	0	0
2	E	1	Total C N 13 8 5	0	0

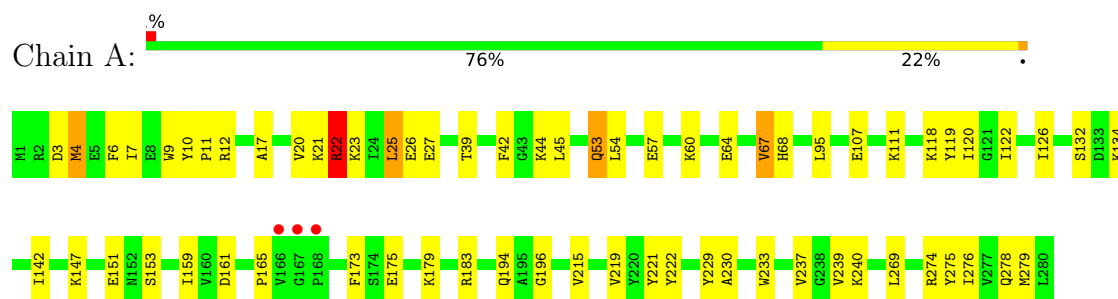
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	168	Total O 168 168	0	0
3	B	187	Total O 187 187	0	0
3	C	140	Total O 140 140	0	0
3	D	148	Total O 148 148	0	0
3	E	164	Total O 164 164	0	0
3	F	123	Total O 123 123	0	0

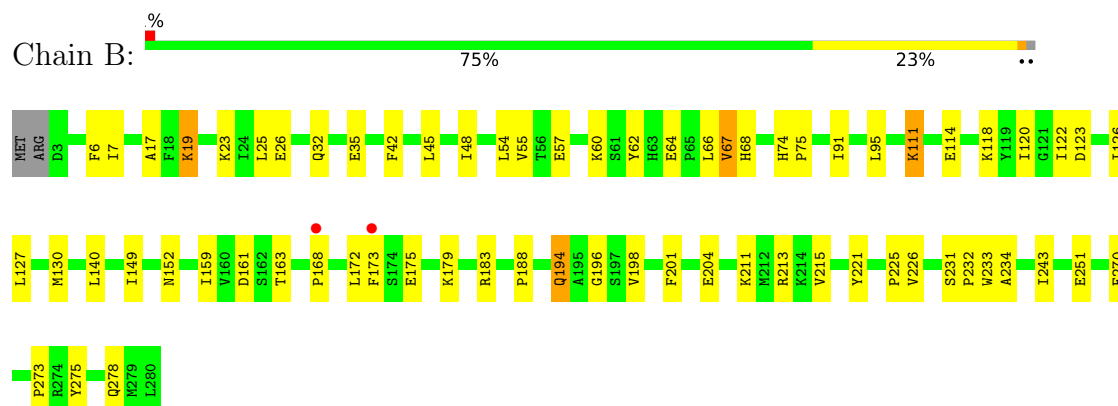
3 Residue-property plots

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.

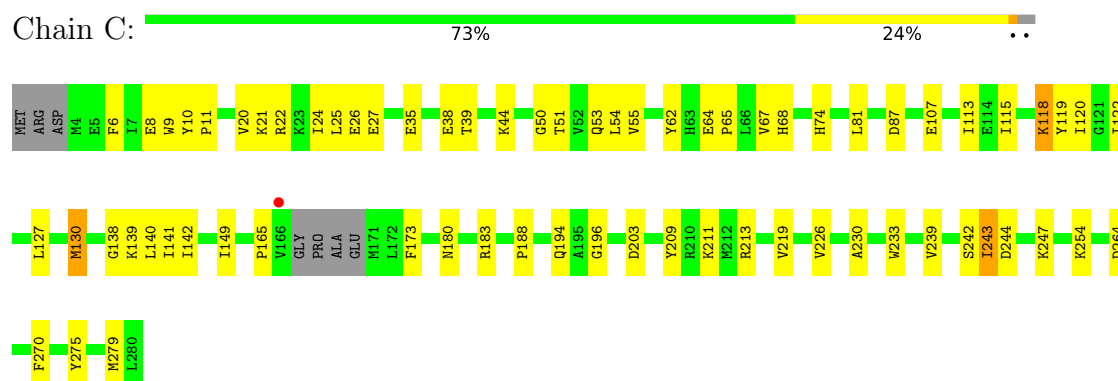
• Molecule 1: spermidine synthase



• Molecule 1: spermidine synthase



• Molecule 1: spermidine synthase



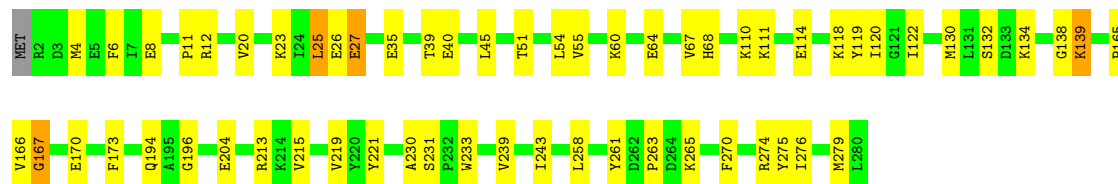
• Molecule 1: spermidine synthase

Chain D:  75% 21% ..



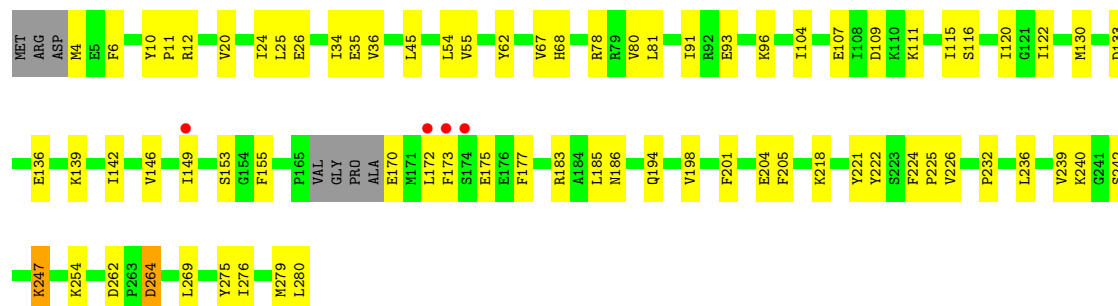
- Molecule 1: spermidine synthase

Chain E:  79% 20% .



- Molecule 1: spermidine synthase

Chain F:  71% 26% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.62Å 81.84Å 96.65Å 99.81° 103.13° 107.85°	Depositor
Resolution (Å)	27.92 – 2.20 27.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (27.92-2.20) 95.9 (27.92-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.248 0.198 , 0.242	Depositor DCC
R_{free} test set	4549 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	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	0.95	EDS
Total number of atoms	14310	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: AG3

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	0.46	0/2309	0.97	9/3110 (0.3%)
1	B	0.49	0/2290	0.96	8/3086 (0.3%)
1	C	0.45	0/2255	0.93	9/3036 (0.3%)
1	D	0.45	0/2240	0.93	6/3014 (0.2%)
1	E	0.47	0/2301	0.94	9/3100 (0.3%)
1	F	0.48	0/2257	0.92	6/3038 (0.2%)
All	All	0.47	0/13652	0.94	47/18384 (0.3%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	VAL	N-CA-C	10.03	120.78	111.45
1	A	215	VAL	N-CA-C	9.41	120.20	111.45
1	F	67	VAL	N-CA-C	9.32	120.12	111.45
1	D	67	VAL	N-CA-C	8.85	120.08	111.67
1	D	215	VAL	N-CA-C	7.58	118.08	111.56
1	B	215	VAL	N-CA-C	7.46	118.06	110.82
1	E	230	ALA	N-CA-C	-7.39	99.08	110.10
1	C	242	SER	N-CA-C	7.18	119.10	111.28
1	A	230	ALA	N-CA-C	-7.15	99.44	110.10
1	A	194	GLN	N-CA-C	-6.81	100.40	110.48
1	E	167	GLY	CA-C-N	6.70	125.94	118.97
1	E	167	GLY	C-N-CA	6.70	125.94	118.97
1	E	270	PHE	N-CA-C	6.70	120.35	112.72
1	C	230	ALA	N-CA-C	-6.58	99.67	109.15
1	D	194	GLN	N-CA-C	-6.50	100.86	110.48
1	C	68	HIS	N-CA-C	6.48	122.36	113.16
1	E	68	HIS	N-CA-C	6.20	121.97	113.16
1	F	68	HIS	N-CA-C	6.17	121.92	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LEU	N-CA-C	6.08	117.79	108.42
1	E	215	VAL	N-CA-C	5.96	117.33	111.67
1	F	186	ASN	N-CA-C	-5.90	103.15	110.41
1	A	68	HIS	N-CA-C	5.80	121.39	113.16
1	B	55	VAL	N-CA-C	-5.79	99.78	108.12
1	E	194	GLN	N-CA-C	-5.78	101.92	110.48
1	A	67	VAL	N-CA-C	5.75	121.30	109.34
1	D	274	ARG	N-CA-C	5.60	117.39	111.28
1	C	194	GLN	N-CA-C	-5.58	101.39	110.20
1	B	19	LYS	N-CA-C	-5.57	101.40	110.20
1	F	136	GLU	N-CA-C	5.53	116.98	111.07
1	B	68	HIS	CA-CB-CG	-5.47	108.33	113.80
1	F	55	VAL	N-CA-C	-5.47	100.24	108.12
1	F	80	VAL	N-CA-C	5.43	116.30	108.48
1	A	3	ASP	N-CA-C	5.42	115.44	108.34
1	B	194	GLN	N-CA-C	-5.38	102.91	110.50
1	B	270	PHE	N-CA-C	5.37	118.94	112.93
1	A	53	GLN	N-CA-C	-5.32	106.47	113.12
1	D	20	VAL	N-CA-C	5.27	115.55	108.17
1	E	67	VAL	N-CA-C	5.25	120.25	109.34
1	B	67	VAL	N-CA-C	5.24	120.25	109.34
1	C	74	HIS	CA-C-N	5.20	124.86	119.56
1	C	74	HIS	C-N-CA	5.20	124.86	119.56
1	C	239	VAL	N-CA-C	5.18	116.82	108.85
1	D	68	HIS	N-CA-C	5.12	120.43	113.16
1	E	274	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	A	22	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	C	270	PHE	N-CA-C	5.05	118.32	112.97
1	B	152	ASN	N-CA-C	5.03	117.61	109.40

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	2256	0	2252	48	0
1	B	2237	0	2227	44	0
1	C	2204	0	2201	59	0
1	D	2190	0	2185	45	0
1	E	2248	0	2240	38	0
1	F	2206	0	2198	53	0
2	A	13	0	21	2	0
2	C	13	0	21	1	0
2	E	13	0	21	0	0
3	A	168	0	0	5	0
3	B	187	0	0	4	0
3	C	140	0	0	2	0
3	D	148	0	0	5	0
3	E	164	0	0	3	0
3	F	123	0	0	3	0
All	All	14310	0	13366	285	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 11.

All (285) 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:C:118:LYS:HE2	1:C:119:TYR:CE1	2.05	0.92
1:A:274:ARG:HD3	3:A:1104:HOH:O	1.73	0.89
1:C:118:LYS:HE2	1:C:119:TYR:CZ	2.14	0.82
1:C:138:GLY:C	1:C:139:LYS:HD2	2.06	0.81
1:E:4:MET:HB3	1:E:20:VAL:HG23	1.64	0.80
1:C:25:LEU:HD11	1:C:27:GLU:HG3	1.67	0.76
1:C:22:ARG:NE	1:C:24:ILE:HD11	2.02	0.75
1:B:130:MET:HG2	1:B:140:LEU:HB2	1.69	0.75
1:D:231:SER:HB2	1:D:232:PRO:HA	1.68	0.75
1:C:118:LYS:CE	1:C:119:TYR:CE1	2.69	0.75
1:F:116:SER:HA	1:F:120:ILE:HG12	1.72	0.69
1:F:104:ILE:HD12	1:F:155:PHE:HE1	1.57	0.69
1:F:146:VAL:O	1:F:149:ILE:HG22	1.92	0.69
1:B:168:PRO:O	1:B:172:LEU:HD23	1.93	0.68
1:C:213:ARG:HG3	1:C:219:VAL:HB	1.76	0.67
1:C:130:MET:HE1	1:C:139:LYS:N	2.09	0.67
1:A:95:LEU:HD12	1:A:126:ILE:HD13	1.77	0.67
1:D:130:MET:HE3	1:D:138:GLY:C	2.19	0.67
1:B:213:ARG:NH1	3:B:389:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ILE:HA	1:E:279:MET:HE2	1.77	0.67
1:F:153:SER:HB3	1:F:183:ARG:HH11	1.58	0.66
1:D:32:GLN:HG3	1:D:48:ILE:HG23	1.78	0.66
1:B:163:THR:HG23	3:B:311:HOH:O	1.96	0.65
1:C:118:LYS:NZ	1:C:119:TYR:HE1	1.94	0.65
1:A:54:LEU:HD12	1:A:54:LEU:C	2.22	0.64
1:A:120:ILE:HG22	1:A:122:ILE:HG23	1.80	0.64
1:C:130:MET:HE1	1:C:138:GLY:C	2.22	0.64
1:C:26:GLU:HG3	1:C:35:GLU:HG2	1.79	0.64
1:A:165:PRO:HB3	1:A:173:PHE:CD1	2.34	0.63
1:B:23:LYS:HE2	1:B:26:GLU:HB2	1.80	0.63
1:C:22:ARG:CZ	1:C:24:ILE:CD1	2.77	0.62
1:A:21:LYS:O	1:A:22:ARG:HB3	2.00	0.62
1:E:25:LEU:C	1:E:25:LEU:HD23	2.25	0.62
1:E:118:LYS:HD2	1:E:119:TYR:CE2	2.35	0.61
1:D:25:LEU:C	1:D:25:LEU:HD12	2.25	0.61
1:A:45:LEU:C	1:A:45:LEU:HD23	2.26	0.60
1:D:133:ASP:O	1:D:134:LYS:HE2	2.01	0.60
1:B:42:PHE:C	1:B:57:GLU:HB2	2.26	0.60
1:D:138:GLY:C	1:D:139:LYS:HD2	2.27	0.60
1:C:54:LEU:C	1:C:54:LEU:HD12	2.27	0.60
1:D:133:ASP:C	1:D:134:LYS:HE2	2.27	0.60
1:C:118:LYS:NZ	1:C:119:TYR:CE1	2.70	0.59
1:E:60:LYS:O	1:E:64:GLU:HB2	2.02	0.59
1:E:54:LEU:C	1:E:54:LEU:HD12	2.27	0.59
1:F:104:ILE:HD12	1:F:155:PHE:CE1	2.38	0.59
1:F:201:PHE:CZ	1:F:204:GLU:HG2	2.38	0.58
1:E:26:GLU:HG3	1:E:35:GLU:HG2	1.84	0.58
1:A:118:LYS:HD2	1:A:119:TYR:CE1	2.39	0.58
1:E:130:MET:HE3	1:E:138:GLY:C	2.29	0.57
1:B:26:GLU:HG3	1:B:35:GLU:HG2	1.85	0.57
1:B:225:PRO:HA	1:B:231:SER:OG	2.04	0.57
1:C:113:ILE:HG23	1:C:127:LEU:HD22	1.86	0.57
1:F:153:SER:HB3	1:F:183:ARG:NH1	2.19	0.57
1:F:45:LEU:C	1:F:45:LEU:HD23	2.30	0.57
1:B:201:PHE:CZ	1:B:204:GLU:HG2	2.40	0.56
1:D:120:ILE:HG22	1:D:122:ILE:HG23	1.87	0.56
1:C:22:ARG:NE	1:C:24:ILE:CD1	2.68	0.56
1:C:118:LYS:HZ1	1:C:119:TYR:HE1	1.54	0.56
1:A:4:MET:HB3	1:A:20:VAL:HG23	1.88	0.55
1:C:21:LYS:O	1:C:22:ARG:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:GLU:HG3	3:E:1104:HOH:O	2.06	0.55
1:A:12:ARG:HG3	1:A:12:ARG:HH11	1.71	0.55
1:D:134:LYS:HE2	1:D:134:LYS:HA	1.87	0.55
1:D:201:PHE:O	1:D:204:GLU:HG2	2.06	0.55
1:D:144:ASP:OD2	1:D:147:LYS:HG2	2.06	0.55
1:F:116:SER:HA	1:F:120:ILE:CG1	2.37	0.55
1:D:224:PHE:CG	1:D:225:PRO:HD2	2.42	0.55
1:A:44:LYS:HD3	1:A:119:TYR:O	2.06	0.54
1:D:183:ARG:HB3	3:D:372:HOH:O	2.05	0.54
1:E:120:ILE:HG22	1:E:122:ILE:HG23	1.89	0.54
1:E:276:ILE:HA	1:E:279:MET:CE	2.36	0.54
1:C:139:LYS:HE2	3:C:1065:HOH:O	2.06	0.54
1:C:8:GLU:HG3	1:C:50:GLY:O	2.07	0.54
1:E:4:MET:HB3	1:E:20:VAL:CG2	2.36	0.54
1:C:139:LYS:HD2	1:C:139:LYS:N	2.22	0.54
1:B:231:SER:OG	1:B:232:PRO:HA	2.09	0.53
1:B:198:VAL:HB	1:B:232:PRO:HG2	1.90	0.53
1:F:221:TYR:CE2	1:F:280:LEU:HD11	2.43	0.53
1:F:54:LEU:HD12	1:F:54:LEU:C	2.33	0.53
1:A:179:LYS:O	1:A:183:ARG:HG3	2.09	0.53
1:F:218:LYS:HB2	1:F:239:VAL:CG2	2.39	0.53
1:E:12:ARG:NH1	3:E:1054:HOH:O	2.41	0.53
1:E:27:GLU:OE1	1:E:111:LYS:HE3	2.09	0.52
1:A:196:GLY:HA2	1:A:233:TRP:CZ2	2.44	0.52
1:B:54:LEU:C	1:B:54:LEU:HD12	2.35	0.52
1:C:20:VAL:HA	1:C:39:THR:HA	1.92	0.52
1:B:114:GLU:O	1:B:118:LYS:HE2	2.10	0.52
1:D:249:ASP:OD1	1:D:251:GLU:HB2	2.10	0.52
1:C:244:ASP:OD2	1:C:247:LYS:HE2	2.10	0.52
1:C:22:ARG:CZ	1:C:24:ILE:HD11	2.40	0.52
1:C:53:GLN:O	1:C:54:LEU:HB3	2.10	0.52
1:A:153:SER:HB3	3:A:1029:HOH:O	2.09	0.52
1:E:239:VAL:CG1	1:E:243:ILE:HB	2.40	0.52
1:C:130:MET:HE1	1:C:139:LYS:CA	2.40	0.51
1:A:132:SER:O	1:A:134:LYS:HG3	2.10	0.51
1:A:222:TYR:HB2	1:A:269:LEU:O	2.10	0.51
1:C:196:GLY:HA2	1:C:233:TRP:CZ2	2.45	0.51
1:C:275:TYR:CD1	1:C:279:MET:HE2	2.46	0.51
1:E:196:GLY:HA2	1:E:233:TRP:CZ2	2.46	0.51
1:A:269:LEU:O	1:A:269:LEU:HG	2.10	0.51
1:B:130:MET:HG2	1:B:140:LEU:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TYR:HB3	1:A:11:PRO:CD	2.42	0.50
1:F:149:ILE:O	1:F:183:ARG:NH2	2.45	0.50
1:C:25:LEU:HD12	1:C:26:GLU:N	2.27	0.50
1:D:10:TYR:HB3	1:D:11:PRO:HD2	1.94	0.50
1:E:6:PHE:CD1	1:E:6:PHE:C	2.89	0.50
1:E:239:VAL:HG11	1:E:243:ILE:HB	1.93	0.50
1:F:222:TYR:HB2	1:F:269:LEU:O	2.12	0.50
1:E:221:TYR:CD1	1:E:221:TYR:C	2.89	0.50
1:C:188:PRO:HB2	1:C:243:ILE:HG13	1.94	0.49
1:D:107:GLU:O	1:D:142:ILE:HA	2.12	0.49
1:B:6:PHE:CD1	1:B:6:PHE:C	2.89	0.49
1:D:275:TYR:HA	1:D:278:GLN:HE21	1.77	0.49
1:F:24:ILE:HB	1:F:36:VAL:HG12	1.94	0.49
1:F:170:GLU:CG	1:F:173:PHE:HB2	2.42	0.49
1:F:275:TYR:O	1:F:279:MET:HG3	2.11	0.49
1:F:109:ASP:OD1	1:F:111:LYS:HB2	2.11	0.49
1:E:231:SER:HA	3:E:1010:HOH:O	2.12	0.49
1:C:254:LYS:NZ	1:C:264:ASP:OD2	2.44	0.49
1:B:173:PHE:O	1:B:211:LYS:NZ	2.46	0.49
1:D:204:GLU:HB3	3:D:293:HOH:O	2.13	0.49
1:B:173:PHE:HZ	1:B:204:GLU:HG3	1.78	0.49
1:D:54:LEU:HD12	1:D:54:LEU:C	2.38	0.49
1:E:45:LEU:HD23	1:E:45:LEU:C	2.37	0.49
1:A:151:GLU:HB3	3:A:1122:HOH:O	2.12	0.49
1:B:66:LEU:HD21	1:B:161:ASP:HB2	1.94	0.49
1:D:197:SER:H	1:D:201:PHE:HD2	1.61	0.49
1:F:183:ARG:C	1:F:183:ARG:HD2	2.38	0.48
1:A:118:LYS:HD2	1:A:119:TYR:CZ	2.48	0.48
1:F:175:GLU:HG3	3:F:314:HOH:O	2.14	0.48
1:C:21:LYS:HB2	1:C:38:GLU:HG3	1.96	0.48
1:D:45:LEU:C	1:D:45:LEU:HD23	2.39	0.48
1:E:165:PRO:HG3	1:E:204:GLU:HG3	1.96	0.48
1:B:91:ILE:O	1:B:95:LEU:HG	2.13	0.48
1:A:107:GLU:O	1:A:142:ILE:HA	2.14	0.48
1:B:275:TYR:HA	1:B:278:GLN:HE21	1.79	0.48
1:A:42:PHE:C	1:A:57:GLU:HB2	2.39	0.48
1:A:60:LYS:O	1:A:64:GLU:HB2	2.14	0.48
1:F:81:LEU:HD12	1:F:104:ILE:O	2.14	0.48
1:A:4:MET:HE3	1:A:4:MET:HA	1.97	0.47
1:A:276:ILE:HA	1:A:279:MET:CE	2.43	0.47
1:C:244:ASP:CG	1:C:247:LYS:HE2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLU:OE1	1:E:258:LEU:HB3	2.14	0.47
1:B:149:ILE:O	1:B:183:ARG:NH2	2.43	0.47
1:C:6:PHE:CD1	1:C:6:PHE:C	2.93	0.47
1:C:107:GLU:O	1:C:142:ILE:HA	2.14	0.47
1:E:132:SER:O	1:E:134:LYS:HG3	2.14	0.47
1:F:130:MET:HE3	1:F:139:LYS:N	2.30	0.47
1:A:12:ARG:HG3	1:A:12:ARG:NH1	2.30	0.47
1:D:95:LEU:HD12	1:D:126:ILE:HD13	1.96	0.47
1:D:134:LYS:HE2	1:D:134:LYS:CA	2.44	0.47
1:F:221:TYR:HE2	1:F:280:LEU:HD11	1.79	0.47
1:A:7:ILE:HG12	1:A:17:ALA:HB2	1.96	0.47
1:A:9:TRP:CE2	1:B:19:LYS:HE3	2.50	0.47
1:E:167:GLY:O	1:E:170:GLU:HB3	2.14	0.46
1:F:4:MET:HE2	1:F:20:VAL:HG11	1.96	0.46
1:D:19:LYS:HB3	1:D:40:GLU:HG3	1.97	0.46
1:D:196:GLY:HA2	1:D:233:TRP:CZ2	2.50	0.46
1:D:229:TYR:N	1:D:229:TYR:CD1	2.83	0.46
1:F:170:GLU:HG2	1:F:173:PHE:HB2	1.96	0.46
1:B:221:TYR:CD1	1:B:221:TYR:C	2.92	0.46
1:C:25:LEU:HD12	1:C:26:GLU:H	1.81	0.46
1:D:66:LEU:HD21	1:D:161:ASP:HB2	1.98	0.46
1:D:229:TYR:N	1:D:229:TYR:HD1	2.14	0.46
1:C:149:ILE:HG22	1:C:180:ASN:HB3	1.97	0.46
1:E:166:VAL:O	1:E:166:VAL:HG13	2.14	0.46
1:E:213:ARG:HA	1:E:219:VAL:HG11	1.98	0.46
1:F:26:GLU:HG3	1:F:35:GLU:HG2	1.98	0.46
1:C:183:ARG:HG3	1:C:183:ARG:HH11	1.81	0.46
1:D:214:LYS:HE2	3:D:298:HOH:O	2.14	0.46
1:A:10:TYR:HB3	1:A:11:PRO:HD2	1.97	0.46
1:C:140:LEU:HD12	1:C:141:ILE:H	1.80	0.46
1:C:209:TYR:CZ	1:C:213:ARG:CD	2.99	0.46
1:D:175:GLU:HG3	3:D:298:HOH:O	2.15	0.46
1:E:130:MET:HE3	1:E:139:LYS:N	2.31	0.46
1:A:27:GLU:OE2	1:A:111:LYS:HD2	2.15	0.45
1:E:261:TYR:O	1:E:263:PRO:HD3	2.15	0.45
1:F:218:LYS:HB2	1:F:239:VAL:HG22	1.97	0.45
1:C:275:TYR:HD1	1:C:279:MET:HE2	1.81	0.45
1:F:6:PHE:CD1	1:F:6:PHE:C	2.95	0.45
1:B:95:LEU:HD12	1:B:126:ILE:HD13	1.98	0.45
1:C:10:TYR:HB3	1:C:11:PRO:HD2	1.98	0.45
1:F:276:ILE:HA	1:F:279:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:TYR:CD1	1:F:221:TYR:C	2.94	0.45
1:F:247:LYS:HB2	1:F:247:LYS:NZ	2.32	0.45
1:C:10:TYR:HB3	1:C:11:PRO:CD	2.47	0.45
1:F:93:GLU:O	1:F:96:LYS:HB2	2.17	0.45
1:F:11:PRO:O	1:F:12:ARG:HB2	2.17	0.45
1:D:251:GLU:HA	1:D:251:GLU:OE1	2.17	0.45
1:C:25:LEU:HD23	1:C:115:ILE:HG23	1.98	0.44
1:C:62:TYR:HB2	1:C:226:VAL:HG13	1.99	0.44
1:C:130:MET:CE	1:C:138:GLY:C	2.90	0.44
1:D:10:TYR:HB3	1:D:11:PRO:CD	2.47	0.44
1:F:120:ILE:HG22	1:F:122:ILE:HG23	1.98	0.44
1:E:165:PRO:HB3	1:E:173:PHE:CD1	2.52	0.44
1:F:25:LEU:O	1:F:35:GLU:HA	2.17	0.44
1:D:146:VAL:O	1:D:149:ILE:HG22	2.18	0.44
1:B:126:ILE:O	1:B:130:MET:HB2	2.18	0.44
1:E:20:VAL:HA	1:E:39:THR:HA	1.99	0.44
1:B:175:GLU:OE1	1:B:179:LYS:HE3	2.18	0.43
1:D:55:VAL:HG23	1:D:55:VAL:O	2.19	0.43
1:B:175:GLU:O	1:B:179:LYS:HG3	2.18	0.43
1:D:103:VAL:HG13	1:D:138:GLY:HA2	1.99	0.43
1:D:265:LYS:HD3	3:D:330:HOH:O	2.17	0.43
1:E:23:LYS:HE2	1:E:26:GLU:HB2	1.99	0.43
1:F:62:TYR:HB2	1:F:226:VAL:CG1	2.48	0.43
1:B:196:GLY:HA2	1:B:233:TRP:CZ2	2.53	0.43
1:F:262:ASP:OD1	1:F:264:ASP:HB2	2.18	0.43
1:A:53:GLN:O	1:A:54:LEU:HB3	2.19	0.43
1:F:198:VAL:HB	1:F:232:PRO:HG2	1.99	0.43
1:A:147:LYS:HA	1:A:147:LYS:HD3	1.78	0.43
1:B:188:PRO:HB2	1:B:243:ILE:HG12	1.99	0.43
1:F:275:TYR:CD2	1:F:279:MET:HE2	2.53	0.43
1:A:9:TRP:CZ3	1:B:19:LYS:HG2	2.54	0.43
1:C:8:GLU:CD	1:C:51:THR:HA	2.44	0.43
1:A:229:TYR:HB3	1:A:233:TRP:CE3	2.53	0.43
1:C:87:ASP:OD2	2:C:1002:AG3:H92	2.19	0.43
1:A:20:VAL:HG12	1:A:39:THR:HG22	2.00	0.43
1:E:275:TYR:O	1:E:279:MET:HG3	2.19	0.43
1:D:139:LYS:HD2	1:D:139:LYS:N	2.34	0.42
1:D:149:ILE:HD12	1:D:149:ILE:HA	1.83	0.42
1:A:6:PHE:CD1	1:A:6:PHE:C	2.97	0.42
1:A:219:VAL:HA	1:A:237:VAL:O	2.19	0.42
1:A:239:VAL:CG1	1:A:240:LYS:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:TYR:O	1:A:279:MET:HG3	2.19	0.42
1:C:209:TYR:CZ	1:C:213:ARG:HD3	2.53	0.42
1:F:107:GLU:O	1:F:142:ILE:HA	2.20	0.42
1:F:172:LEU:HD23	1:F:177:PHE:CZ	2.54	0.42
1:E:11:PRO:O	1:E:12:ARG:HB2	2.19	0.42
1:B:32:GLN:HG3	1:B:48:ILE:HG23	2.00	0.42
1:C:81:LEU:CD2	1:C:149:ILE:HD11	2.50	0.42
1:C:118:LYS:CE	1:C:119:TYR:CZ	2.94	0.42
1:C:119:TYR:CD1	1:C:119:TYR:N	2.87	0.42
1:A:23:LYS:HE2	1:A:26:GLU:HB2	2.02	0.42
1:C:64:GLU:N	1:C:65:PRO:HD2	2.35	0.42
1:B:7:ILE:HG12	1:B:17:ALA:HB2	2.00	0.42
1:F:91:ILE:HD13	1:F:130:MET:SD	2.60	0.42
1:B:60:LYS:O	1:B:64:GLU:HB2	2.19	0.42
1:B:45:LEU:C	1:B:45:LEU:HD23	2.44	0.42
1:B:123:ASP:CG	1:B:127:LEU:HG	2.44	0.42
1:C:120:ILE:HG22	1:C:122:ILE:HG23	2.02	0.42
1:C:211:LYS:HE2	3:C:1029:HOH:O	2.20	0.42
1:D:154:GLY:HA2	1:D:186:ASN:OD1	2.19	0.42
1:E:110:LYS:O	1:E:114:GLU:HG3	2.20	0.42
1:B:62:TYR:HB2	1:B:226:VAL:HG13	2.02	0.42
1:C:55:VAL:HG23	1:C:55:VAL:O	2.20	0.42
1:F:183:ARG:HD2	1:F:183:ARG:O	2.20	0.42
1:C:165:PRO:HB3	1:C:173:PHE:CD1	2.55	0.41
1:B:211:LYS:HE2	3:B:436:HOH:O	2.20	0.41
1:C:9:TRP:CE3	1:D:19:LYS:HE3	2.55	0.41
1:A:67:VAL:HG22	1:A:159:ILE:HD13	2.00	0.41
1:A:161:ASP:OD1	2:A:1001:AG3:H72	2.20	0.41
1:D:218:LYS:HD2	1:D:220:TYR:OH	2.20	0.41
1:F:78:ARG:NH2	3:F:366:HOH:O	2.52	0.41
1:F:224:PHE:CG	1:F:225:PRO:HD2	2.55	0.41
1:A:25:LEU:HG	1:A:26:GLU:N	2.36	0.41
1:F:81:LEU:HB2	1:F:155:PHE:CD1	2.55	0.41
1:F:149:ILE:HG21	1:F:177:PHE:CE1	2.55	0.41
1:B:120:ILE:HG22	1:B:122:ILE:HG23	2.02	0.41
1:D:201:PHE:HB3	1:D:204:GLU:HG2	2.03	0.41
1:A:42:PHE:O	1:A:57:GLU:HB2	2.21	0.41
1:B:67:VAL:HG22	1:B:159:ILE:HD13	2.02	0.41
1:D:19:LYS:CB	1:D:40:GLU:HG3	2.50	0.41
1:D:75:PRO:O	1:D:76:ASN:HB2	2.21	0.41
1:F:205:PHE:CE1	1:F:236:LEU:HD21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:O	1:A:278:GLN:HG3	2.21	0.41
1:E:8:GLU:CD	1:E:51:THR:HA	2.46	0.41
1:E:265:LYS:HD3	3:F:351:HOH:O	2.20	0.41
1:F:10:TYR:HB3	1:F:11:PRO:CD	2.51	0.41
1:F:34:ILE:HD13	1:F:115:ILE:HD12	2.01	0.41
1:A:175:GLU:HB2	3:A:1056:HOH:O	2.21	0.40
1:B:74:HIS:ND1	1:B:75:PRO:HD2	2.36	0.40
1:B:163:THR:HA	3:B:409:HOH:O	2.21	0.40
1:F:185:LEU:HB2	1:F:240:LYS:HD2	2.03	0.40
1:A:221:TYR:CD1	1:A:221:TYR:C	2.99	0.40
1:B:25:LEU:O	1:B:35:GLU:HA	2.22	0.40
1:B:111:LYS:HE3	1:B:111:LYS:HA	2.03	0.40
1:B:198:VAL:HG22	1:B:234:ALA:HB2	2.03	0.40
1:C:44:LYS:HD2	1:C:119:TYR:O	2.21	0.40
1:D:147:LYS:HA	1:D:147:LYS:HD3	1.90	0.40
1:F:254:LYS:HE2	1:F:254:LYS:HB3	1.89	0.40
2:A:1001:AG3:HB2	3:A:1024:HOH:O	2.21	0.40
1:E:55:VAL:O	1:E:55:VAL:HG23	2.20	0.40
1:A:7:ILE:HG12	1:A:17:ALA:CB	2.51	0.40
1:F:276:ILE:HA	1:F:279:MET:CE	2.52	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	278/280 (99%)	266 (96%)	12 (4%)	0	100	100
1	B	276/280 (99%)	266 (96%)	10 (4%)	0	100	100
1	C	269/280 (96%)	254 (94%)	14 (5%)	1 (0%)	30	34
1	D	267/280 (95%)	255 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	277/280 (99%)	267 (96%)	10 (4%)	0	100	100
1	F	269/280 (96%)	258 (96%)	10 (4%)	1 (0%)	30	34
All	All	1636/1680 (97%)	1566 (96%)	68 (4%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	243	ILE
1	F	242	SER

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	240/240 (100%)	238 (99%)	2 (1%)	73	85
1	B	238/240 (99%)	234 (98%)	4 (2%)	53	69
1	C	235/240 (98%)	232 (99%)	3 (1%)	61	76
1	D	233/240 (97%)	226 (97%)	7 (3%)	36	49
1	E	239/240 (100%)	236 (99%)	3 (1%)	61	76
1	F	235/240 (98%)	231 (98%)	4 (2%)	53	69
All	All	1420/1440 (99%)	1397 (98%)	23 (2%)	55	71

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	22	ARG
1	B	111	LYS
1	B	194	GLN
1	B	251	GLU
1	B	273	PRO
1	C	118	LYS
1	C	130	MET

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Mol	Chain	Res	Type
1	C	203	ASP
1	D	32	GLN
1	D	33	LYS
1	D	103	VAL
1	D	128	GLU
1	D	198	VAL
1	D	229	TYR
1	D	264	ASP
1	E	25	LEU
1	E	27	GLU
1	E	139	LYS
1	F	133	ASP
1	F	194	GLN
1	F	247	LYS
1	F	264	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	B	76	ASN
1	B	278	GLN
1	C	76	ASN
1	C	278	GLN
1	D	28	GLN
1	D	278	GLN
1	E	76	ASN
1	E	278	GLN
1	F	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	AG3	A	1001	-	12,12,12	1.16	1 (8%)	11,12,12	0.76	0
2	AG3	C	1002	-	12,12,12	0.98	1 (8%)	11,12,12	0.93	0
2	AG3	E	1003	-	12,12,12	1.06	1 (8%)	11,12,12	0.91	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	AG3	A	1001	-	-	2/10/10/10	-
2	AG3	C	1002	-	-	2/10/10/10	-
2	AG3	E	1003	-	-	1/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	AG3	CZ-NE	3.26	1.39	1.33
2	E	1003	AG3	CZ-NE	2.69	1.38	1.33
2	C	1002	AG3	CZ-NE	2.61	1.38	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1002	AG3	N-CA-CB-CG
2	C	1002	AG3	CB-CA-N-C7
2	A	1001	AG3	NE-CD-CG-CB
2	A	1001	AG3	CA-CB-CG-CD
2	E	1003	AG3	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	AG3	2	0
2	C	1002	AG3	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	280/280 (100%)	-0.15	3 (1%) 78 76	18, 29, 46, 64	0
1	B	278/280 (99%)	-0.29	2 (0%) 84 82	14, 26, 45, 56	0
1	C	273/280 (97%)	-0.02	1 (0%) 88 87	20, 32, 54, 61	0
1	D	271/280 (96%)	-0.21	1 (0%) 88 87	16, 30, 48, 63	0
1	E	279/280 (99%)	-0.28	0 100 100	17, 28, 45, 54	0
1	F	273/280 (97%)	-0.02	4 (1%) 72 69	17, 31, 48, 63	0
All	All	1654/1680 (98%)	-0.16	11 (0%) 84 82	14, 29, 48, 64	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	173	PHE	3.6
1	B	173	PHE	3.3
1	A	168	PRO	3.2
1	A	166	VAL	2.8
1	B	168	PRO	2.7
1	C	166	VAL	2.4
1	F	174	SER	2.1
1	F	149	ILE	2.1
1	A	167	GLY	2.1
1	F	172	LEU	2.0
1	D	22	ARG	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
2	AG3	C	1002	13/13	0.87	0.11	31,33,34,36	0
2	AG3	A	1001	13/13	0.91	0.10	20,25,31,31	0
2	AG3	E	1003	13/13	0.93	0.08	24,26,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.