



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:10 PM UTC

PDB ID : 2E9X / pdb_00002e9x
Title : The crystal structure of human GINS core complex
Authors : Kamada, K.; Hanaoka, F.
Deposited on : 2007-01-27
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<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

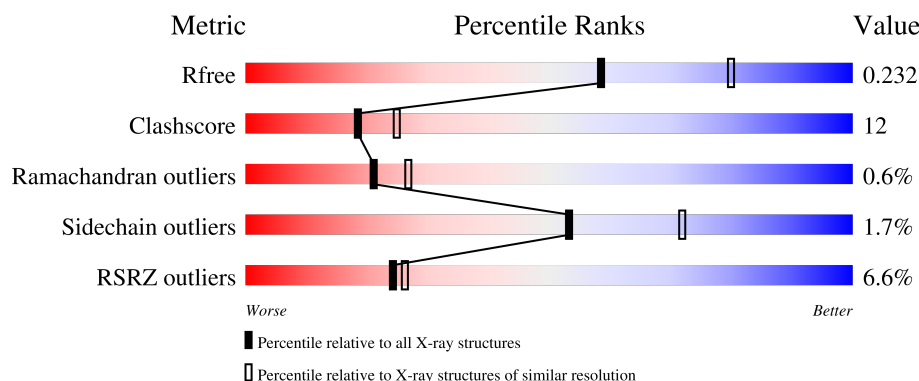
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

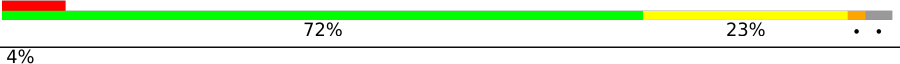
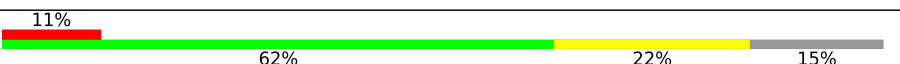
The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	149	
1	E	149	
2	B	185	
2	F	185	
3	C	219	

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Mol	Chain	Length	Quality of chain
3	G	219	7% 64% 17% • 16%
4	D	223	4% 61% 26% 12%
4	H	223	6% 61% 26% • 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11975 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 DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1181	740	216	215	10			
1	E	144	Total	C	N	O	S	0	0	0
			1181	740	216	215	10			

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1424	911	241	263	9			
2	F	175	Total	C	N	O	S	0	0	0
			1424	911	241	263	9			

- Molecule 3 is a protein called GINS complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	186	Total	C	N	O	S	0	0	0
			1488	945	257	279	7			
3	G	183	Total	C	N	O	S	0	0	0
			1467	932	252	276	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	998	GLY	-	cloning artifact	UNP Q9BRX5
C	999	PRO	-	cloning artifact	UNP Q9BRX5
C	1000	HIS	-	cloning artifact	UNP Q9BRX5
G	-2	GLY	-	cloning artifact	UNP Q9BRX5
G	-1	PRO	-	cloning artifact	UNP Q9BRX5
G	0	HIS	-	cloning artifact	UNP Q9BRX5

- Molecule 4 is a protein called GINS complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1624	1032	274	308	10			
4	H	197	Total	C	N	O	S	0	0	0
			1624	1032	274	308	10			

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		
6	B	53	Total	O	0	0
			53	53		

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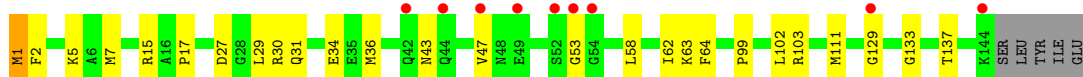
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	60	Total 60	O 60	0	0
6	D	89	Total 89	O 89	0	0
6	E	54	Total 54	O 54	0	0
6	F	74	Total 74	O 74	0	0
6	G	67	Total 67	O 67	0	0
6	H	84	Total 84	O 84	0	0

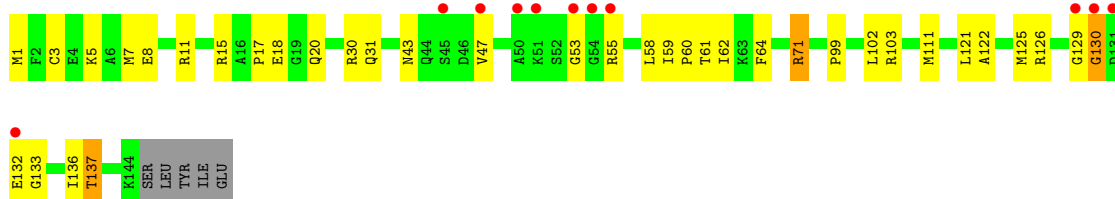
3 Residue-property plots [i](#)

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.

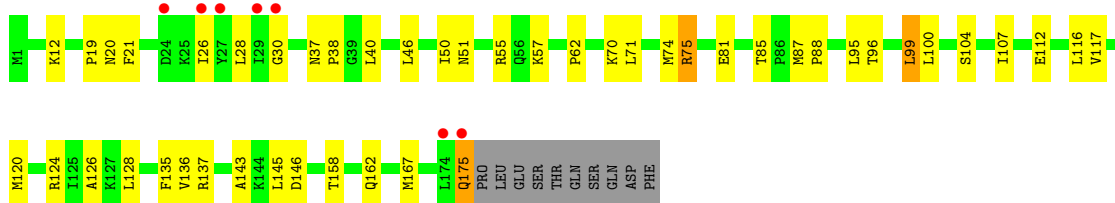
- Molecule 1: DNA replication complex GINS protein PSF1



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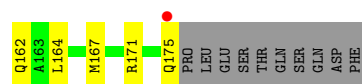


- Molecule 2: DNA replication complex GINS protein PSF2

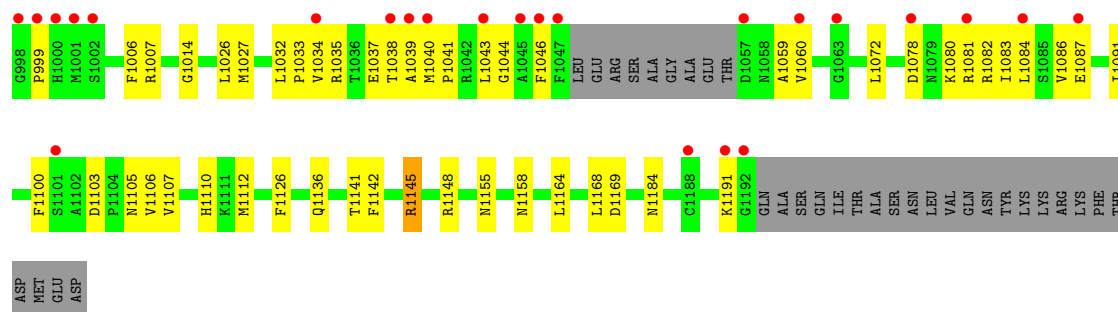


- Molecule 2: DNA replication complex GINS protein PSF2

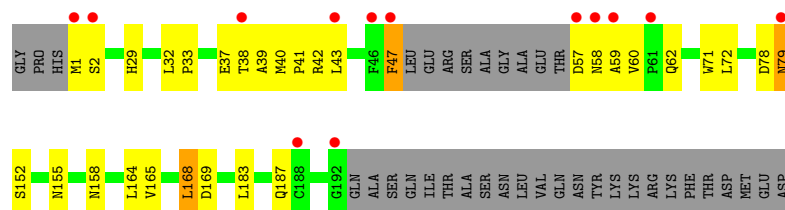




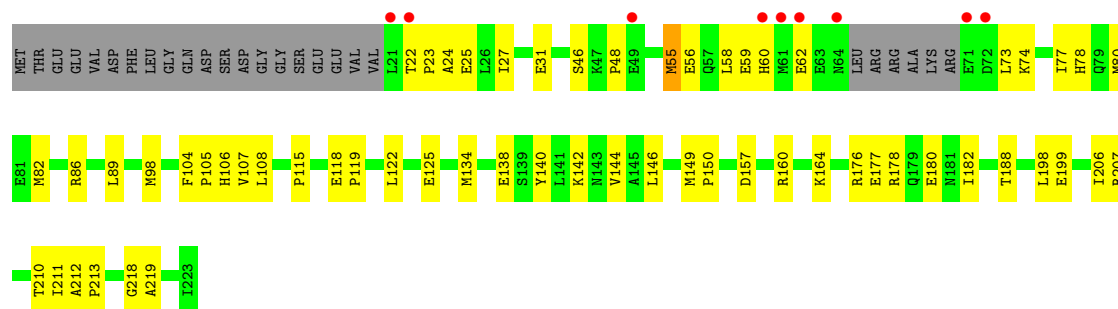
• Molecule 3: GINS complex subunit 3



• Molecule 3: GINS complex subunit 3

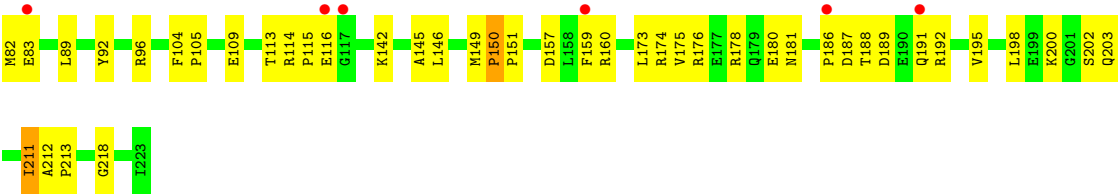


• Molecule 4: GINS complex subunit 4



• Molecule 4: GINS complex subunit 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.93Å 88.74Å 102.13Å 104.69° 102.96° 95.47°	Depositor
Resolution (Å)	29.82 – 2.30 29.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.82-2.30) 97.4 (29.82-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.233 0.195 , 0.232	Depositor DCC
R_{free} test set	4042 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1204	0.80	1/1617 (0.1%)
1	E	0.38	0/1204	0.83	1/1617 (0.1%)
2	B	0.39	0/1454	0.86	2/1969 (0.1%)
2	F	0.38	0/1454	0.84	2/1969 (0.1%)
3	C	0.37	0/1524	0.91	3/2056 (0.1%)
3	G	0.38	0/1501	0.86	3/2024 (0.1%)
4	D	0.40	0/1655	0.86	2/2231 (0.1%)
4	H	0.39	0/1655	0.84	5/2231 (0.2%)
All	All	0.38	0/11651	0.85	19/15714 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	ASP	N-CA-C	8.80	123.02	111.75
2	F	157	GLY	N-CA-C	6.86	120.94	112.64
3	C	1014	GLY	CA-C-N	6.75	126.26	119.24
3	C	1014	GLY	C-N-CA	6.75	126.26	119.24
1	E	137	THR	N-CA-C	-6.65	105.17	113.28
1	A	137	THR	N-CA-C	-6.19	105.49	113.16
2	B	126	ALA	N-CA-C	-5.98	104.84	111.36
3	G	107	VAL	N-CA-C	5.59	116.82	109.21
3	G	98	THR	N-CA-C	-5.53	105.33	111.36
3	G	110	HIS	N-CA-C	-5.52	104.67	111.40
4	H	211	ILE	N-CA-C	5.47	117.37	112.17
4	H	150	PRO	CA-C-N	5.36	126.55	119.84
4	H	150	PRO	C-N-CA	5.36	126.55	119.84
4	D	150	PRO	CA-C-N	5.28	126.44	119.84
4	D	150	PRO	C-N-CA	5.28	126.44	119.84
3	C	1110	HIS	N-CA-C	-5.26	104.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	146	ASP	N-CA-C	5.25	117.74	111.71
4	H	47	LYS	CA-C-N	5.12	124.57	119.24
4	H	47	LYS	C-N-CA	5.12	124.57	119.24

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	1181	0	1173	19	0
1	E	1181	0	1173	35	0
2	B	1424	0	1449	40	0
2	F	1424	0	1449	31	0
3	C	1488	0	1436	43	0
3	G	1467	0	1422	34	0
4	D	1624	0	1631	46	0
4	H	1624	0	1631	55	0
5	A	15	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	H	5	0	0	0	0
6	A	51	0	0	0	0
6	B	53	0	0	1	0
6	C	60	0	0	0	0
6	D	89	0	0	0	0
6	E	54	0	0	1	0
6	F	74	0	0	1	0
6	G	67	0	0	0	0
6	H	84	0	0	1	0
All	All	11975	0	11364	273	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 12.

All (273) 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:E:125:MET:HE1	1:E:137:THR:HG23	1.43	0.98
2:B:26:ILE:HG22	4:D:74:LYS:HE2	1.48	0.96
2:F:74:MET:SD	2:F:88:PRO:HG3	2.06	0.95
2:B:74:MET:SD	2:B:88:PRO:HG3	2.13	0.89
3:C:1184:ASN:HD22	4:H:191:GLN:HE21	1.22	0.88
2:B:175:GLN:H	2:B:175:GLN:NE2	1.73	0.87
3:C:999:PRO:HG3	2:F:171:ARG:HH22	1.41	0.86
3:G:40:MET:HB2	3:G:60:VAL:HG12	1.56	0.86
3:C:1034:VAL:HG11	3:C:1084:LEU:HD23	1.59	0.82
2:B:62:PRO:HG3	2:B:107:ILE:HD13	1.63	0.81
4:D:22:THR:HG22	4:D:24:ALA:H	1.46	0.80
2:F:62:PRO:HG3	2:F:107:ILE:HD13	1.64	0.79
3:G:33:PRO:HB2	3:G:87:GLU:HB3	1.65	0.79
1:A:99:PRO:HD2	1:A:102:LEU:HD12	1.64	0.78
3:C:1091:ILE:HG23	3:C:1112:MET:HE2	1.66	0.77
4:H:37:GLU:HG3	4:H:92:TYR:HE1	1.49	0.77
3:C:999:PRO:HG3	2:F:171:ARG:NH2	2.00	0.75
4:D:55:MET:HE2	4:D:55:MET:HA	1.69	0.74
2:B:175:GLN:HB2	4:D:188:THR:HG21	1.68	0.74
1:E:129:GLY:H	1:E:133:GLY:HA2	1.54	0.73
3:C:1041:PRO:HA	3:C:1059:ALA:HB2	1.69	0.73
4:H:55:MET:HA	4:H:55:MET:HE2	1.70	0.72
1:E:125:MET:HE1	1:E:137:THR:CG2	2.19	0.72
4:D:77:ILE:HA	4:D:80:MET:HE3	1.71	0.72
1:E:103:ARG:HG2	1:E:111:MET:CE	2.20	0.71
1:E:121:LEU:HD11	1:E:125:MET:HE3	1.71	0.71
4:H:181:ASN:HA	4:H:195:VAL:CG1	2.21	0.71
4:D:142:LYS:HA	4:D:146:LEU:HB2	1.71	0.70
1:E:43:ASN:O	1:E:47:VAL:HG23	1.91	0.70
3:C:1037:GLU:HG3	3:C:1081:ARG:HB3	1.74	0.69
1:E:125:MET:HE2	1:E:136:ILE:CG1	2.22	0.69
2:F:136:VAL:HG13	2:F:167:MET:SD	2.33	0.69
4:D:22:THR:HB	4:D:25:GLU:HG3	1.72	0.69
1:A:129:GLY:H	1:A:133:GLY:HA2	1.57	0.69
2:B:87:MET:HE2	2:B:87:MET:HA	1.75	0.69
3:G:165:VAL:HA	3:G:168:LEU:HD22	1.75	0.67
2:B:175:GLN:H	2:B:175:GLN:HE21	1.43	0.67
4:D:157:ASP:OD2	4:D:160:ARG:HG3	1.94	0.67
4:H:21:LEU:HD11	4:H:29:ARG:NH1	2.10	0.67
3:G:41:PRO:HA	3:G:59:ALA:HB2	1.77	0.67
4:H:72:ASP:HA	4:H:75:VAL:HG22	1.77	0.66
2:B:75:ARG:HH11	2:B:75:ARG:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1103:ASP:O	3:C:1106:VAL:HG12	1.96	0.65
4:D:27:ILE:O	4:D:31:GLU:HG3	1.96	0.65
1:E:122:ALA:O	1:E:126:ARG:HG3	1.97	0.65
4:H:37:GLU:HG3	4:H:92:TYR:CE1	2.31	0.65
1:A:64:PHE:CE1	3:C:1072:LEU:HD21	2.32	0.64
2:F:23:LEU:HD11	4:H:74:LYS:HE2	1.78	0.64
3:G:155:ASN:HD21	3:G:158:ASN:HA	1.60	0.64
1:A:30:ARG:O	1:A:34:GLU:HG3	1.97	0.64
1:A:1:MET:HB3	3:C:1046:PHE:CD1	2.33	0.64
4:D:108:LEU:HD12	4:D:134:MET:HE2	1.79	0.63
4:H:116:GLU:H	4:H:116:GLU:CD	2.07	0.63
3:C:1083:ILE:HG22	3:C:1084:LEU:HD12	1.80	0.63
2:B:75:ARG:HB3	2:B:75:ARG:NH1	2.14	0.63
3:C:1105:ASN:HD21	3:C:1145:ARG:HA	1.64	0.63
4:H:142:LYS:HA	4:H:146:LEU:HB2	1.81	0.62
1:E:99:PRO:HD2	1:E:102:LEU:HD12	1.82	0.62
4:H:178:ARG:HH12	4:H:180:GLU:CG	2.12	0.62
1:A:27:ASP:O	1:A:31:GLN:HG3	2.00	0.62
3:C:1041:PRO:HA	3:C:1059:ALA:CB	2.30	0.62
1:E:125:MET:HE2	1:E:136:ILE:HG12	1.82	0.61
3:G:152:SER:OG	3:G:164:LEU:HD13	2.00	0.61
4:H:46:SER:C	4:H:48:PRO:HD3	2.25	0.61
3:C:1040:MET:HB3	3:C:1043:LEU:HD12	1.83	0.60
4:D:107:VAL:HG12	4:D:122:LEU:HD11	1.84	0.60
2:F:60:LEU:HD12	2:F:103:ALA:HB2	1.83	0.60
3:G:155:ASN:ND2	3:G:158:ASN:HA	2.16	0.59
2:B:55:ARG:HB3	2:B:57:LYS:HE3	1.84	0.59
2:F:87:MET:HE1	2:F:120:MET:HE2	1.84	0.59
2:B:74:MET:CE	2:B:88:PRO:HG3	2.32	0.59
3:C:1141:THR:O	3:C:1145:ARG:HG2	2.03	0.59
4:D:55:MET:HE3	4:D:89:LEU:CD2	2.32	0.59
1:E:121:LEU:CD1	1:E:125:MET:HE3	2.32	0.58
4:D:104:PHE:CG	4:D:105:PRO:HD3	2.38	0.58
4:H:175:VAL:HG21	4:H:198:LEU:HB3	1.86	0.58
3:C:1100:PHE:CZ	3:C:1107:VAL:HG11	2.38	0.58
1:A:1:MET:HE2	1:A:2:PHE:H	1.69	0.57
2:B:120:MET:O	2:B:124:ARG:HG3	2.04	0.57
3:C:1184:ASN:ND2	4:H:191:GLN:HE21	1.99	0.57
4:H:113:THR:HG22	4:H:113:THR:O	2.02	0.57
4:D:178:ARG:NH1	4:D:199:GLU:OE1	2.38	0.57
1:E:3:CYS:HA	6:E:1007:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1006:PHE:CZ	4:D:98:MET:HG3	2.39	0.57
4:H:157:ASP:OD2	4:H:160:ARG:HG3	2.04	0.56
4:H:178:ARG:HH12	4:H:180:GLU:CD	2.13	0.56
2:F:40:LEU:HD12	2:F:41:PRO:HD2	1.86	0.56
3:C:1083:ILE:C	3:C:1084:LEU:HD12	2.31	0.56
1:E:103:ARG:HG2	1:E:111:MET:HE1	1.86	0.56
4:D:58:LEU:O	4:D:62:GLU:HG2	2.06	0.56
1:E:103:ARG:HG2	1:E:111:MET:HE3	1.86	0.56
1:A:1:MET:HB3	3:C:1046:PHE:CG	2.40	0.56
1:A:1:MET:HE3	1:A:64:PHE:CZ	2.41	0.56
2:B:135:PHE:CE1	2:B:143:ALA:HB2	2.40	0.56
3:G:81:ARG:H	3:G:81:ARG:HD2	1.71	0.55
4:H:178:ARG:HH12	4:H:180:GLU:HG3	1.72	0.55
3:C:1148:ARG:HG2	3:C:1148:ARG:HH11	1.71	0.55
3:G:78:ASP:OD2	3:G:82:ARG:HB3	2.05	0.55
4:H:55:MET:HE3	4:H:89:LEU:CD2	2.37	0.55
3:C:1044:GLY:HA2	3:C:1060:VAL:HG22	1.89	0.55
1:E:7:MET:HE2	3:G:29:HIS:CG	2.42	0.55
1:A:36:MET:SD	4:D:149:MET:HE2	2.46	0.55
1:E:125:MET:HE2	1:E:136:ILE:HG13	1.87	0.55
2:B:51:ASN:HD21	2:B:55:ARG:HE	1.54	0.55
2:F:17:ILE:HG22	2:F:60:LEU:HD23	1.89	0.54
1:E:58:LEU:O	1:E:62:ILE:HG13	2.07	0.54
2:B:158:THR:O	2:B:162:GLN:HG3	2.07	0.54
4:D:107:VAL:HG11	4:D:122:LEU:HD21	1.89	0.54
3:G:40:MET:HB2	3:G:60:VAL:CG1	2.34	0.54
1:A:47:VAL:HG22	1:A:62:ILE:HD13	1.89	0.53
3:G:81:ARG:HG2	3:G:85:SER:HB3	1.89	0.53
4:D:22:THR:HG23	4:D:23:PRO:HD2	1.88	0.53
2:F:137:ARG:HG2	6:F:1036:HOH:O	2.07	0.53
4:H:37:GLU:OE2	4:H:96:ARG:NH1	2.37	0.53
2:B:120:MET:O	2:B:124:ARG:CG	2.57	0.53
3:C:1083:ILE:HG22	3:C:1084:LEU:CD1	2.38	0.53
4:D:182:ILE:HG13	4:D:198:LEU:HG	1.91	0.52
3:C:1034:VAL:HG11	3:C:1084:LEU:CD2	2.34	0.52
4:D:56:GLU:HG2	4:D:60:HIS:CD2	2.44	0.52
1:A:43:ASN:O	1:A:47:VAL:HG23	2.09	0.52
2:B:74:MET:HE1	2:B:88:PRO:HG3	1.91	0.51
1:E:121:LEU:CG	1:E:125:MET:HE3	2.40	0.51
4:D:107:VAL:CG1	4:D:122:LEU:HD21	2.40	0.51
4:H:22:THR:OG1	4:H:25:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:42:ARG:HG3	3:G:42:ARG:HH11	1.75	0.51
4:D:82:MET:O	4:D:86:ARG:HG3	2.11	0.51
4:D:134:MET:O	4:D:138:GLU:HG3	2.11	0.51
1:E:5:LYS:HD3	1:E:31:GLN:HB3	1.93	0.51
4:D:212:ALA:HB3	4:D:213:PRO:HD3	1.93	0.50
4:H:173:LEU:C	4:H:173:LEU:HD12	2.36	0.50
2:F:128:LEU:HD23	2:F:128:LEU:O	2.11	0.50
4:H:104:PHE:CG	4:H:105:PRO:HD3	2.47	0.50
2:B:124:ARG:HB2	6:B:205:HOH:O	2.11	0.50
2:B:136:VAL:HG13	2:B:167:MET:SD	2.52	0.50
1:E:55:ARG:HG3	1:E:58:LEU:HG	1.92	0.50
4:H:55:MET:HE3	4:H:89:LEU:HD23	1.94	0.50
4:H:178:ARG:NH1	4:H:180:GLU:HG3	2.25	0.50
2:F:141:ALA:CB	4:H:186:PRO:HA	2.42	0.50
3:G:32:LEU:HD21	3:G:86:VAL:CG1	2.41	0.50
1:A:5:LYS:HE2	1:A:31:GLN:OE1	2.12	0.49
1:A:58:LEU:O	1:A:62:ILE:HG13	2.12	0.49
4:H:78:HIS:O	4:H:82:MET:HG2	2.12	0.49
1:A:103:ARG:HG2	1:A:111:MET:HE1	1.93	0.49
2:B:145:LEU:N	2:B:145:LEU:HD23	2.26	0.49
3:C:1086:VAL:HG21	3:C:1126:PHE:CD2	2.48	0.49
1:E:129:GLY:O	1:E:130:GLY:C	2.55	0.49
4:H:55:MET:CE	4:H:58:LEU:HD12	2.43	0.49
4:D:55:MET:HE3	4:D:89:LEU:HD23	1.95	0.49
2:F:51:ASN:O	2:F:55:ARG:HG3	2.11	0.49
4:D:177:GLU:HB2	4:D:219:ALA:HA	1.95	0.49
1:E:71:ARG:HG3	3:G:71:TRP:CD2	2.48	0.49
1:E:59:ILE:HB	1:E:60:PRO:HD3	1.94	0.48
2:F:62:PRO:HG3	2:F:107:ILE:CD1	2.40	0.48
2:B:70:LYS:O	2:B:74:MET:HG3	2.13	0.48
4:H:79:GLN:O	4:H:83:GLU:HG3	2.13	0.48
3:G:86:VAL:HG21	3:G:126:PHE:CD2	2.49	0.48
4:H:55:MET:O	4:H:59:GLU:HG3	2.12	0.48
1:A:7:MET:HE1	3:C:1026:LEU:HD23	1.94	0.48
2:B:51:ASN:ND2	4:D:80:MET:HE1	2.28	0.48
2:F:175:GLN:NE2	4:H:188:THR:OG1	2.46	0.48
4:D:106:HIS:CE1	4:D:164:LYS:HG2	2.49	0.48
1:E:53:GLY:C	1:E:55:ARG:H	2.21	0.48
4:D:55:MET:HA	4:D:55:MET:CE	2.43	0.47
1:E:64:PHE:CE1	3:G:72:LEU:HD21	2.48	0.47
3:G:60:VAL:HG13	3:G:60:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:218:GLY:HA2	6:H:1074:HOH:O	2.14	0.47
4:H:181:ASN:HA	4:H:195:VAL:HG11	1.95	0.47
3:C:1034:VAL:HG12	3:C:1035:ARG:N	2.29	0.47
4:D:22:THR:HG22	4:D:24:ALA:N	2.22	0.47
3:G:80:LYS:O	3:G:81:ARG:C	2.57	0.47
2:B:100:LEU:O	2:B:104:SER:HB3	2.15	0.46
3:C:1033:PRO:HB2	3:C:1087:GLU:HB3	1.97	0.46
3:G:38:THR:C	3:G:62:GLN:HB3	2.39	0.46
2:B:96:THR:HG21	2:B:117:VAL:HG21	1.95	0.46
4:H:109:GLU:HB2	4:H:159:PHE:CE2	2.50	0.46
4:D:104:PHE:CD2	4:D:105:PRO:HD3	2.50	0.46
4:D:115:PRO:HD2	4:D:118:GLU:OE2	2.15	0.46
2:F:60:LEU:HD12	2:F:103:ALA:CB	2.44	0.46
1:E:55:ARG:NH2	3:G:57:ASP:OD1	2.48	0.46
4:D:62:GLU:OE1	4:D:82:MET:HE1	2.16	0.46
4:H:72:ASP:CA	4:H:75:VAL:HG22	2.46	0.46
2:B:112:GLU:O	2:B:116:LEU:HD13	2.15	0.46
4:D:206:ILE:HG12	4:D:207:ARG:N	2.31	0.45
1:E:8:GLU:OE2	1:E:11:ARG:NH1	2.48	0.45
4:D:178:ARG:NH2	4:D:180:GLU:OE2	2.50	0.45
2:B:167:MET:HG3	3:C:1142:PHE:CE2	2.52	0.45
2:F:74:MET:HB3	2:F:120:MET:HE1	1.97	0.45
3:C:1080:LYS:HB2	3:C:1082:ARG:HG3	1.98	0.45
3:G:41:PRO:C	3:G:43:LEU:H	2.25	0.45
4:H:104:PHE:CD2	4:H:105:PRO:HD3	2.52	0.45
4:D:46:SER:C	4:D:48:PRO:HD3	2.42	0.45
4:H:173:LEU:O	4:H:203:GLN:HA	2.17	0.45
1:A:1:MET:HE3	1:A:64:PHE:CE2	2.51	0.44
2:F:23:LEU:HD21	2:F:26:ILE:HD11	1.99	0.44
3:C:1080:LYS:HD2	3:C:1082:ARG:HE	1.81	0.44
4:H:186:PRO:HG3	4:H:192:ARG:HB3	2.00	0.44
2:B:71:LEU:HB2	2:B:116:LEU:HD23	1.99	0.44
3:C:1038:THR:HG22	3:C:1039:ALA:N	2.33	0.44
3:C:1155:ASN:OD1	3:C:1158:ASN:HA	2.18	0.44
2:B:95:LEU:O	2:B:99:LEU:HB2	2.17	0.44
3:G:37:GLU:HG3	3:G:81:ARG:HB3	1.99	0.44
2:F:87:MET:HE1	2:F:120:MET:CE	2.48	0.44
2:F:141:ALA:HB2	4:H:186:PRO:HA	1.98	0.44
4:D:73:LEU:O	4:D:77:ILE:HG13	2.17	0.43
2:F:75:ARG:NH1	2:F:76:ASP:OD1	2.51	0.43
3:C:1148:ARG:HG2	3:C:1148:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:ASN:HB2	4:H:80:MET:HE1	2.00	0.43
4:H:187:ASP:OD1	4:H:189:ASP:HB3	2.18	0.43
4:H:189:ASP:OD2	4:H:192:ARG:HG3	2.18	0.43
2:B:12:LYS:HB3	2:B:12:LYS:HE2	1.85	0.43
2:B:81:GLU:HG3	2:B:85:THR:HG22	2.00	0.43
2:B:167:MET:HG3	3:C:1142:PHE:HE2	1.83	0.43
4:D:140:TYR:O	4:D:144:VAL:HG12	2.18	0.43
1:E:1:MET:HE1	3:G:47:PHE:HE2	1.83	0.43
3:G:38:THR:HG22	3:G:39:ALA:N	2.33	0.43
3:C:1078:ASP:OD2	3:C:1082:ARG:HB2	2.18	0.43
3:G:81:ARG:N	3:G:81:ARG:CD	2.81	0.43
4:H:150:PRO:HA	4:H:151:PRO:HD3	1.87	0.43
2:B:19:PRO:HD2	2:B:40:LEU:O	2.18	0.43
2:B:46:LEU:O	2:B:50:ILE:HG12	2.17	0.43
2:B:28:LEU:HD23	4:D:78:HIS:CE1	2.54	0.43
4:D:59:GLU:O	4:D:62:GLU:HB2	2.19	0.43
1:E:17:PRO:HG2	1:E:20:GLN:NE2	2.33	0.43
1:E:129:GLY:N	1:E:133:GLY:HA2	2.29	0.43
2:F:158:THR:O	2:F:162:GLN:HG3	2.19	0.43
2:B:55:ARG:O	2:B:57:LYS:HG3	2.19	0.42
1:E:18:GLU:OE1	3:G:1:MET:HE2	2.20	0.42
3:G:81:ARG:HG2	3:G:85:SER:CB	2.49	0.42
1:E:61:THR:HG23	3:G:43:LEU:HG	2.00	0.42
4:H:21:LEU:HD11	4:H:29:ARG:HH11	1.82	0.42
4:D:176:ARG:HG3	4:D:218:GLY:O	2.19	0.42
2:F:40:LEU:HD12	2:F:41:PRO:CD	2.49	0.42
2:F:160:LEU:O	2:F:164:LEU:HG	2.20	0.42
2:F:61:LEU:HA	2:F:62:PRO:HD3	1.90	0.42
4:H:212:ALA:HB3	4:H:213:PRO:HD3	2.01	0.42
1:E:15:ARG:O	1:E:17:PRO:HD3	2.20	0.42
4:H:61:MET:HG2	4:H:82:MET:SD	2.60	0.42
3:G:84:LEU:O	3:G:84:LEU:HD12	2.19	0.41
3:G:183:LEU:O	3:G:187:GLN:HG3	2.19	0.41
2:B:20:ASN:OD1	2:B:20:ASN:C	2.64	0.41
2:B:74:MET:C	2:B:120:MET:HE1	2.45	0.41
3:C:1164:LEU:O	3:C:1168:LEU:HG	2.20	0.41
4:H:72:ASP:HA	4:H:75:VAL:CG2	2.48	0.41
4:H:114:ARG:HA	4:H:115:PRO:HD3	1.83	0.41
4:H:211:ILE:HD12	4:H:211:ILE:C	2.44	0.41
1:A:15:ARG:O	1:A:17:PRO:HD3	2.20	0.41
2:B:21:PHE:CD2	2:B:57:LYS:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:LEU:HG	1:E:125:MET:HE3	2.03	0.41
3:C:1141:THR:O	3:C:1145:ARG:CG	2.67	0.41
4:H:176:ARG:O	4:H:200:LYS:HE2	2.20	0.41
3:C:1032:LEU:HD12	3:C:1033:PRO:HD2	2.03	0.41
3:C:1086:VAL:HG21	3:C:1126:PHE:CE2	2.55	0.41
2:F:29:ILE:CD1	4:H:82:MET:HE1	2.50	0.41
4:H:174:ARG:HA	4:H:202:SER:O	2.20	0.41
3:C:1027:MET:SD	3:C:1027:MET:C	3.04	0.41
1:E:30:ARG:NH1	1:E:30:ARG:HB3	2.35	0.41
2:F:103:ALA:O	2:F:107:ILE:HG12	2.21	0.41
3:G:32:LEU:HD21	3:G:86:VAL:HG13	2.02	0.41
4:H:72:ASP:C	4:H:75:VAL:HG22	2.46	0.41
4:D:55:MET:CE	4:D:58:LEU:HD12	2.51	0.41
4:D:211:ILE:C	4:D:211:ILE:HD12	2.46	0.41
4:D:118:GLU:HG3	4:D:119:PRO:HD2	2.02	0.40
4:H:115:PRO:O	4:H:116:GLU:C	2.65	0.40
3:G:78:ASP:O	3:G:79:ASN:C	2.63	0.40
2:B:37:ASN:HA	2:B:38:PRO:HD3	1.97	0.40
1:A:63:LYS:HE2	1:A:63:LYS:HB3	1.86	0.40
2:B:30:GLY:HA2	4:D:24:ALA:CB	2.52	0.40
3:C:1035:ARG:NH1	3:C:1037:GLU:OE2	2.54	0.40
2:F:89:SER:HA	2:F:90:PRO:HD3	1.95	0.40
3:G:42:ARG:HG3	3:G:42:ARG:NH1	2.37	0.40
4:H:145:ALA:O	4:H:149:MET:HG3	2.21	0.40
3:C:1007:ARG:HH11	3:C:1007:ARG:HG3	1.86	0.40
2:F:66:MET:HG2	2:F:113:ILE:HD13	2.04	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	142/149 (95%)	135 (95%)	6 (4%)	1 (1%)	18	23
1	E	142/149 (95%)	135 (95%)	5 (4%)	2 (1%)	9	9
2	B	173/185 (94%)	168 (97%)	5 (3%)	0	100	100
2	F	173/185 (94%)	170 (98%)	3 (2%)	0	100	100
3	C	182/219 (83%)	173 (95%)	8 (4%)	1 (0%)	24	31
3	G	179/219 (82%)	170 (95%)	5 (3%)	4 (2%)	5	4
4	D	193/223 (86%)	186 (96%)	7 (4%)	0	100	100
4	H	193/223 (86%)	187 (97%)	6 (3%)	0	100	100
All	All	1377/1552 (89%)	1324 (96%)	45 (3%)	8 (1%)	21	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	2	SER
3	G	81	ARG
1	E	130	GLY
1	E	132	GLU
3	C	1191	LYS
3	G	79	ASN
1	A	53	GLY
3	G	58	ASN

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	125/130 (96%)	123 (98%)	2 (2%)	55	73
1	E	125/130 (96%)	124 (99%)	1 (1%)	73	86
2	B	159/169 (94%)	154 (97%)	5 (3%)	35	52
2	F	159/169 (94%)	155 (98%)	4 (2%)	42	60
3	C	160/188 (85%)	157 (98%)	3 (2%)	50	69
3	G	158/188 (84%)	155 (98%)	3 (2%)	50	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	183/205 (89%)	180 (98%)	3 (2%)	55	73
4	H	183/205 (89%)	183 (100%)	0	100	100
All	All	1252/1384 (90%)	1231 (98%)	21 (2%)	53	72

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	LEU
2	B	75	ARG
2	B	99	LEU
2	B	128	LEU
2	B	137	ARG
2	B	175	GLN
3	C	1136	GLN
3	C	1145	ARG
3	C	1169	ASP
4	D	55	MET
4	D	125	GLU
4	D	210	THR
1	E	71	ARG
2	F	25	LYS
2	F	69	GLU
2	F	81	GLU
2	F	145	LEU
3	G	47	PHE
3	G	168	LEU
3	G	169	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	20	GLN
1	A	66	HIS
2	B	51	ASN
2	B	54	GLN
2	B	102	HIS
2	B	139	GLN
2	B	175	GLN

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Mol	Chain	Res	Type
3	C	1058	ASN
3	C	1079	ASN
3	C	1105	ASN
3	C	1136	GLN
3	C	1140	GLN
3	C	1184	ASN
4	D	57	GLN
4	D	78	HIS
1	E	20	GLN
1	E	42	GLN
1	E	48	ASN
1	E	66	HIS
2	F	37	ASN
2	F	54	GLN
2	F	102	HIS
2	F	138	GLN
2	F	175	GLN
3	G	131	ASN
3	G	177	GLN
3	G	184	ASN
3	G	187	GLN
4	H	32	GLN
4	H	57	GLN
4	H	64	ASN
4	H	78	HIS
4	H	143	ASN
4	H	154	GLN
4	H	191	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
5	SO4	A	1002	-	4,4,4	0.38	0	6,6,6	0.08	0
5	SO4	A	1001	-	4,4,4	0.39	0	6,6,6	0.08	0
5	SO4	H	1004	-	4,4,4	0.37	0	6,6,6	0.08	0
5	SO4	F	1005	-	4,4,4	0.37	0	6,6,6	0.07	0
5	SO4	E	1006	-	4,4,4	0.38	0	6,6,6	0.07	0
5	SO4	A	1003	-	4,4,4	0.35	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	144/149 (96%)	0.19	9 (6%) 26 28	16, 32, 71, 83	0
1	E	144/149 (96%)	0.30	11 (7%) 20 21	19, 34, 75, 91	0
2	B	175/185 (94%)	0.20	7 (4%) 42 44	18, 35, 54, 67	0
2	F	175/185 (94%)	0.00	3 (1%) 69 70	18, 29, 54, 62	0
3	C	186/219 (84%)	0.44	24 (12%) 7 8	18, 33, 74, 80	0
3	G	183/219 (83%)	0.29	16 (8%) 16 17	17, 29, 78, 84	0
4	D	197/223 (88%)	0.05	9 (4%) 37 39	16, 29, 58, 93	0
4	H	197/223 (88%)	0.14	14 (7%) 22 24	16, 30, 60, 82	0
All	All	1401/1552 (90%)	0.20	93 (6%) 24 26	16, 32, 69, 93	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	175	GLN	4.9
3	G	1	MET	4.7
3	C	998	GLY	4.6
4	H	64	ASN	4.6
3	G	58	ASN	4.1
4	D	64	ASN	4.1
4	H	49	GLU	4.0
2	F	175	GLN	3.7
3	G	81	ARG	3.7
4	H	60	HIS	3.6
1	E	54	GLY	3.5
1	E	53	GLY	3.3
3	G	43	LEU	3.3
2	B	26	ILE	3.3
3	G	80	LYS	3.3
4	D	61	MET	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	1191	LYS	3.2
3	C	1045	ALA	3.2
3	C	1000	HIS	3.2
1	E	51	LYS	3.1
3	G	47	PHE	3.1
3	G	79	ASN	3.1
1	A	52	SER	3.1
1	A	53	GLY	3.0
3	G	192	GLY	3.0
3	G	2	SER	3.0
1	E	129	GLY	3.0
3	C	1084	LEU	2.9
3	C	1038	THR	2.9
3	G	46	PHE	2.9
1	A	47	VAL	2.9
3	G	38	THR	2.8
3	C	1081	ARG	2.7
3	C	1047	PHE	2.7
1	A	42	GLN	2.7
3	C	1063	GLY	2.7
1	E	47	VAL	2.6
1	A	54	GLY	2.6
3	C	1034	VAL	2.6
3	C	1043	LEU	2.6
1	E	45	SER	2.6
4	H	117	GLY	2.5
4	H	59	GLU	2.5
1	E	130	GLY	2.5
3	C	1192	GLY	2.5
4	H	186	PRO	2.5
1	E	131	ASP	2.5
3	C	1039	ALA	2.5
4	D	60	HIS	2.5
3	G	127	ASP	2.4
3	C	999	PRO	2.4
1	A	129	GLY	2.4
4	D	21	LEU	2.4
4	H	73	LEU	2.4
2	B	24	ASP	2.4
1	A	144	LYS	2.4
2	B	29	ILE	2.4
3	C	1188	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	62	GLU	2.4
4	H	83	GLU	2.3
4	H	159	PHE	2.3
3	C	1057	ASP	2.3
4	D	72	ASP	2.3
4	H	61	MET	2.3
2	F	26	ILE	2.3
3	C	1078	ASP	2.3
1	E	132	GLU	2.3
4	D	49	GLU	2.3
4	D	71	GLU	2.3
4	H	191	GLN	2.2
1	E	55	ARG	2.2
1	E	50	ALA	2.2
3	C	1060	VAL	2.2
3	G	57	ASP	2.2
3	C	1040	MET	2.2
3	C	1087	GLU	2.2
1	A	44	GLN	2.2
2	F	25	LYS	2.2
2	B	30	GLY	2.2
3	C	1002	SER	2.2
3	C	1101	SER	2.1
3	G	59	ALA	2.1
1	A	49	GLU	2.1
3	C	1001	MET	2.1
2	B	174	LEU	2.1
4	H	52	GLU	2.1
2	B	27	TYR	2.1
3	C	1046	PHE	2.1
4	D	22	THR	2.0
3	G	188	CYS	2.0
4	H	116	GLU	2.0
4	H	21	LEU	2.0
3	G	61	PRO	2.0

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

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
5	SO4	A	1002	5/5	0.83	0.14	92,93,93,94	0
5	SO4	A	1001	5/5	0.86	0.15	71,72,73,73	0
5	SO4	H	1004	5/5	0.86	0.09	94,94,94,94	0
5	SO4	E	1006	5/5	0.89	0.16	77,79,79,79	0
5	SO4	F	1005	5/5	0.89	0.14	79,79,79,80	0
5	SO4	A	1003	5/5	0.89	0.12	67,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.