



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:12 PM UTC

PDB ID : 4GMJ / pdb_00004gmj
Title : Structure of human NOT1 MIF4G domain co-crystallized with CAF1
Authors : Petit, P.; Weichenrieder, O.; Wohlbold, L.; Izaurralde, E.
Deposited on : 2012-08-16
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

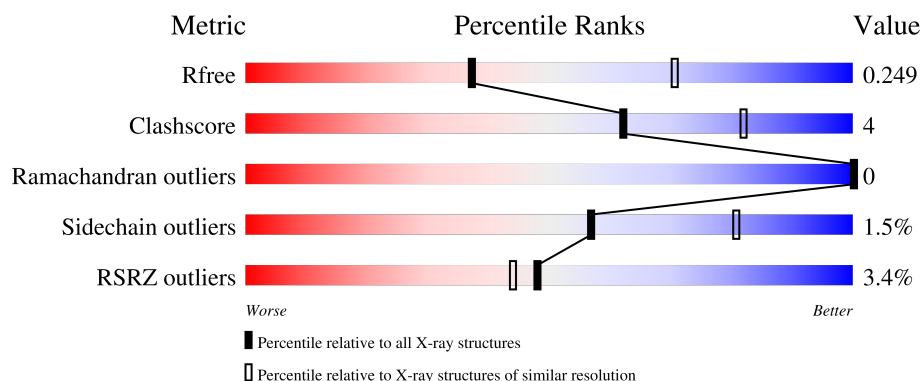
1 Overall quality at a glance

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))
R_{free}	180053	3538 (2.70-2.70)
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	2% 86% 13% .
1	C	229	7% 88% 10% .
1	E	229	3% 92% 8%
2	B	285	2% 80% 12% 7%
2	D	285	3% 80% 11% 9%

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Mol	Chain	Length	Quality of chain
2	F	285	2% 82% 9% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23850 atoms, of which 11741 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 CCR4-NOT transcription complex subunit 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	229	Total	C	H	N	O	S	0	0	0
			3764	1198	1905	310	342	9			
1	C	225	Total	C	H	N	O	S	0	0	0
			3665	1169	1849	303	336	8			
1	E	229	Total	C	H	N	O	S	0	0	0
			3727	1191	1879	307	341	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	HIS	-	expression tag	UNP A5YKK6
A	1090	MET	-	expression tag	UNP A5YKK6
A	1091	LEU	-	expression tag	UNP A5YKK6
A	1092	GLU	-	expression tag	UNP A5YKK6
C	1089	HIS	-	expression tag	UNP A5YKK6
C	1090	MET	-	expression tag	UNP A5YKK6
C	1091	LEU	-	expression tag	UNP A5YKK6
C	1092	GLU	-	expression tag	UNP A5YKK6
E	1089	HIS	-	expression tag	UNP A5YKK6
E	1090	MET	-	expression tag	UNP A5YKK6
E	1091	LEU	-	expression tag	UNP A5YKK6
E	1092	GLU	-	expression tag	UNP A5YKK6

- Molecule 2 is a protein called CCR4-NOT transcription complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	264	Total	C	H	N	O	S	0	0	0
			4182	1372	2045	341	409	15			
2	D	259	Total	C	H	N	O	S	0	0	0
			4139	1360	2027	336	401	15			
2	F	260	Total	C	H	N	O	S	0	0	0
			4109	1354	2012	331	397	15			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	D	2	Total	Mg	0	0
			2	2		
3	F	3	Total	Mg	0	0
			3	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

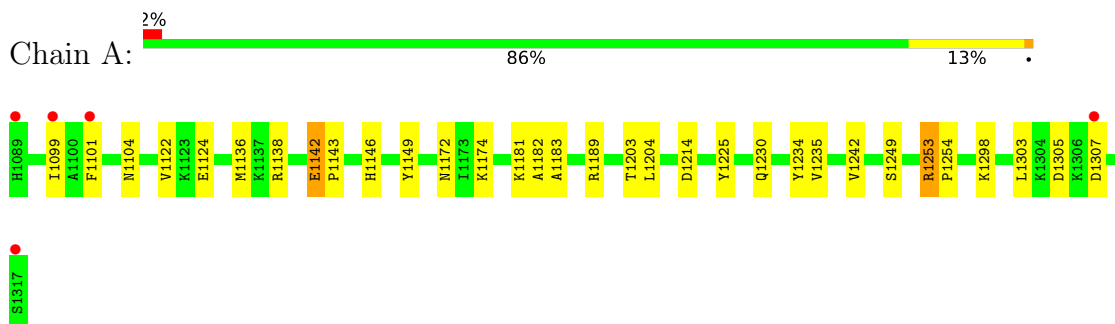
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total 27	O 27	0	0
6	B	64	Total 64	O 64	0	0
6	C	22	Total 22	O 22	0	0
6	D	30	Total 30	O 30	0	0
6	E	19	Total 19	O 19	0	0
6	F	49	Total 49	O 49	0	0

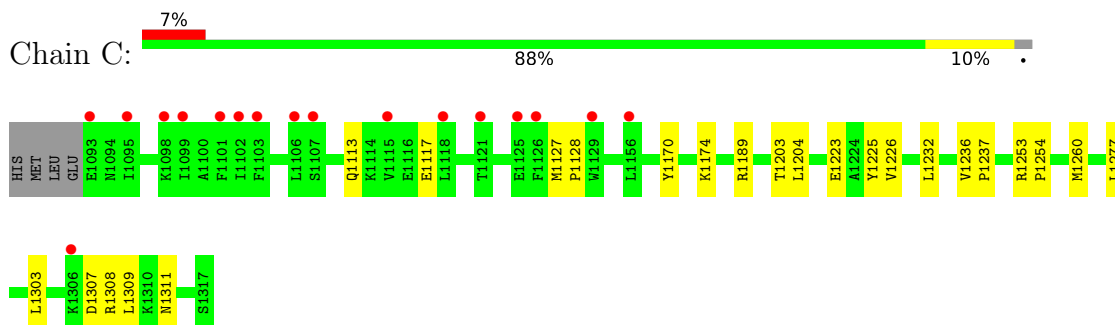
3 Residue-property plots [i](#)

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.

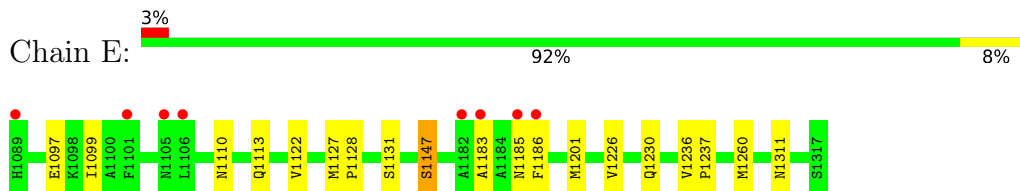
- Molecule 1: CCR4-NOT transcription complex subunit 1



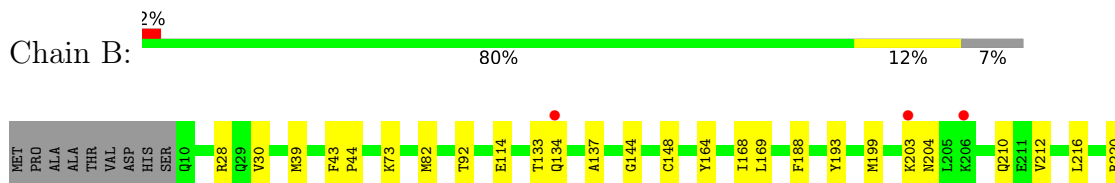
- Molecule 1: CCR4-NOT transcription complex subunit 1

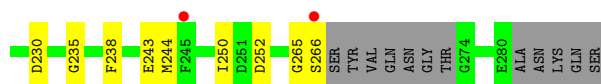


- Molecule 1: CCR4-NOT transcription complex subunit 1

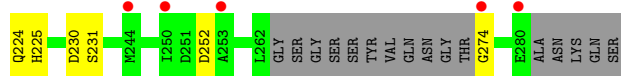
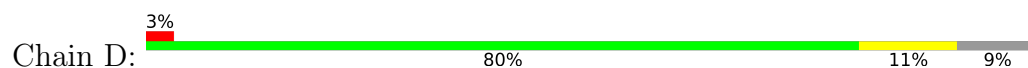


- Molecule 2: CCR4-NOT transcription complex subunit 7

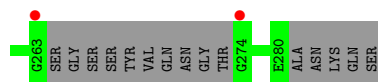
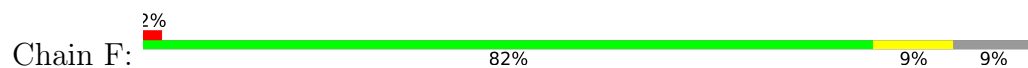




- Molecule 2: CCR4-NOT transcription complex subunit 7



- Molecule 2: CCR4-NOT transcription complex subunit 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.47Å 101.74Å 142.20Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	76.70 – 2.70 76.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (76.70-2.70) 95.2 (76.70-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.214 , 0.249 0.211 , 0.249	Depositor DCC
R_{free} test set	3204 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23850	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: GOL, CL, MG

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	0/1894	0.80	5/2562 (0.2%)
1	C	0.32	0/1850	0.68	0/2505
1	E	0.31	0/1883	0.66	0/2550
2	B	0.34	0/2185	0.71	0/2947
2	D	0.30	0/2160	0.65	2/2913 (0.1%)
2	F	0.31	0/2145	0.66	2/2894 (0.1%)
All	All	0.33	0/12117	0.70	9/16371 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1253	ARG	CA-C-N	-5.78	114.43	120.38
1	A	1253	ARG	C-N-CA	-5.78	114.43	120.38
1	A	1142	GLU	CA-C-N	5.48	125.09	119.56
1	A	1142	GLU	C-N-CA	5.48	125.09	119.56
1	A	1235	VAL	N-CA-C	5.46	116.32	111.90
2	F	222	GLY	CA-C-N	5.24	125.40	119.90
2	F	222	GLY	C-N-CA	5.24	125.40	119.90
2	D	222	GLY	CA-C-N	5.12	125.03	119.76
2	D	222	GLY	C-N-CA	5.12	125.03	119.76

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	1859	1905	1899	19	0
1	C	1816	1849	1844	16	0
1	E	1848	1879	1873	12	0
2	B	2137	2045	2040	18	0
2	D	2112	2027	2027	20	0
2	F	2097	2012	2007	13	0
3	B	3	0	0	0	0
3	D	2	0	0	0	0
3	F	3	0	0	0	0
4	B	6	8	8	0	0
4	D	6	8	8	1	0
4	F	6	8	8	0	0
5	B	1	0	0	1	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	27	0	0	0	0
6	B	64	0	0	0	0
6	C	22	0	0	0	0
6	D	30	0	0	2	0
6	E	19	0	0	0	0
6	F	49	0	0	0	0
All	All	12109	11741	11714	97	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 4.

All (97) 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)
2:D:38:ALA:HB3	2:D:80:THR:HB	1.38	1.00
2:D:40:ASP:OD2	6:D:403:HOH:O	1.98	0.81
2:D:38:ALA:HB1	2:D:231:SER:O	1.87	0.74
1:E:1183:ALA:N	1:E:1230:GLN:OE1	2.27	0.67
2:D:37:VAL:HG11	2:D:153:TRP:CZ3	2.29	0.67
2:B:210:GLN:OE1	2:B:220:ARG:NH1	2.28	0.66
1:C:1307:ASP:O	1:C:1311:ASN:ND2	2.32	0.63
2:F:254:LYS:HG2	2:F:255:TYR:CZ	2.34	0.63
1:A:1181:LYS:C	1:A:1230:GLN:NE2	2.60	0.60
2:B:220:ARG:NH2	2:B:230:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:ARG:NH2	2:D:230:ASP:OD1	2.34	0.59
2:D:274:GLY:N	6:D:410:HOH:O	2.36	0.59
1:E:1099:ILE:HG22	1:E:1122:VAL:HG21	1.84	0.59
1:C:1113:GLN:NE2	1:C:1117:GLU:OE2	2.36	0.58
2:F:220:ARG:NH2	2:F:230:ASP:OD1	2.38	0.56
2:D:43:PHE:O	4:D:303:GOL:H32	2.08	0.54
2:B:82:MET:HE1	2:B:235:GLY:CA	2.38	0.53
1:A:1203:THR:OG1	1:A:1204:LEU:N	2.41	0.53
1:A:1183:ALA:O	1:A:1189:ARG:NH2	2.42	0.53
1:C:1225:TYR:CD2	1:C:1303:LEU:HD22	2.45	0.52
2:B:114:GLU:OE2	1:C:1189:ARG:NH1	2.43	0.52
2:F:65:LEU:C	2:F:65:LEU:HD23	2.35	0.52
2:D:43:PHE:HB2	2:D:44:PRO:CD	2.40	0.52
2:D:199:MET:SD	2:D:212:VAL:HG21	2.50	0.51
2:F:254:LYS:HG2	2:F:255:TYR:CE2	2.45	0.51
1:A:1225:TYR:CG	1:A:1303:LEU:HD22	2.45	0.51
2:F:43:PHE:HB2	2:F:44:PRO:CD	2.40	0.51
2:F:199:MET:SD	2:F:212:VAL:HG21	2.52	0.50
2:B:243:GLU:HG3	2:B:244:MET:N	2.26	0.50
2:F:210:GLN:OE1	2:F:220:ARG:NH1	2.44	0.50
2:D:65:LEU:C	2:D:65:LEU:HD23	2.37	0.50
2:B:164:TYR:O	2:B:168:ILE:HG12	2.12	0.49
1:C:1170:TYR:O	1:C:1174:LYS:HG3	2.12	0.49
2:B:265:GLY:O	2:B:266:SER:C	2.55	0.49
2:D:37:VAL:HG11	2:D:153:TRP:CH2	2.48	0.48
1:C:1127:MET:N	1:C:1128:PRO:CD	2.77	0.48
2:B:73:LYS:HA	5:B:304:CL:CL	2.51	0.47
1:A:1099:ILE:HG22	1:A:1122:VAL:HG21	1.96	0.47
1:A:1142:GLU:OE1	1:A:1149:TYR:OH	2.27	0.47
1:A:1305:ASP:O	1:A:1307:ASP:N	2.42	0.47
2:B:203:LYS:O	2:B:204:ASN:HB2	2.15	0.47
1:E:1230:GLN:HA	1:E:1230:GLN:HE21	1.78	0.46
2:D:202:CYS:CB	2:D:205:LEU:HD12	2.46	0.46
1:A:1136:MET:HE3	1:A:1172:ASN:OD1	2.15	0.46
2:B:199:MET:SD	2:B:212:VAL:HG21	2.55	0.46
2:B:43:PHE:HB2	2:B:44:PRO:CD	2.46	0.46
1:A:1253:ARG:O	1:A:1254:PRO:C	2.56	0.46
1:E:1230:GLN:HA	1:E:1230:GLN:NE2	2.31	0.46
1:A:1249:SER:O	1:A:1253:ARG:HB2	2.16	0.45
1:E:1260:MET:HA	1:E:1260:MET:HE2	1.98	0.45
1:C:1236:VAL:HB	1:C:1237:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1127:MET:HA	1:C:1127:MET:HE2	1.98	0.45
2:F:16:TRP:CZ2	2:F:125:LYS:HD3	2.52	0.45
2:F:36:TYR:CZ	2:F:152:LYS:HD2	2.52	0.45
2:B:144:GLY:HA2	2:B:148:CYS:SG	2.57	0.44
2:B:169:LEU:HD13	2:B:188:PHE:CD1	2.51	0.44
2:F:203:LYS:O	2:F:204:ASN:CB	2.65	0.44
1:A:1138:ARG:O	1:A:1142:GLU:HG2	2.17	0.44
1:A:1181:LYS:HG2	1:A:1234:TYR:CZ	2.53	0.44
2:B:137:ALA:HB2	2:B:168:ILE:HG22	1.99	0.44
2:D:220:ARG:HH12	2:D:224:GLN:HG3	1.83	0.44
2:D:108:TYR:CD1	2:D:113:ILE:HG13	2.53	0.43
2:D:155:SER:HB2	2:D:158:SER:HB3	1.99	0.43
1:E:1127:MET:N	1:E:1128:PRO:CD	2.81	0.43
1:C:1260:MET:HA	1:C:1260:MET:HE2	2.00	0.43
1:A:1182:ALA:N	1:A:1230:GLN:NE2	2.67	0.43
1:A:1225:TYR:CD2	1:A:1303:LEU:HD22	2.53	0.43
1:C:1225:TYR:CG	1:C:1303:LEU:HD22	2.53	0.43
1:E:1147:SER:HA	1:E:1201:MET:HE1	2.01	0.43
2:D:193:TYR:OH	2:D:252:ASP:OD1	2.25	0.43
1:C:1203:THR:OG1	1:C:1204:LEU:N	2.51	0.43
1:C:1253:ARG:HG2	1:C:1254:PRO:O	2.19	0.42
1:A:1181:LYS:C	1:A:1230:GLN:HE22	2.26	0.42
2:D:224:GLN:HG2	2:D:225:HIS:ND1	2.35	0.42
1:A:1143:PRO:HA	1:A:1146:HIS:CE1	2.54	0.42
2:F:54:PHE:O	2:F:57:ASN:HB2	2.19	0.42
2:B:133:THR:HB	2:B:168:ILE:HD12	2.02	0.42
1:E:1236:VAL:HB	1:E:1237:PRO:HD3	2.01	0.42
1:C:1223:GLU:O	1:C:1226:VAL:HG22	2.19	0.42
2:D:39:MET:HA	2:D:78:GLY:O	2.20	0.42
2:B:193:TYR:OH	2:B:252:ASP:OD1	2.27	0.42
2:B:238:PHE:CZ	2:B:250:ILE:CD1	3.03	0.42
1:E:1110:ASN:OD1	1:E:1110:ASN:C	2.62	0.42
1:A:1101:PHE:HA	1:A:1104:ASN:HB2	2.02	0.41
1:E:1186:PHE:CD1	1:E:1186:PHE:C	2.98	0.41
1:E:1185:ASN:O	1:E:1186:PHE:HB3	2.20	0.41
2:F:109:ALA:O	2:F:110:GLN:C	2.62	0.41
2:D:220:ARG:NH1	2:D:224:GLN:HG3	2.35	0.41
1:E:1311:ASN:OD1	1:E:1311:ASN:N	2.54	0.41
2:B:39:MET:SD	2:B:39:MET:C	3.03	0.41
1:C:1170:TYR:O	1:C:1174:LYS:CG	2.69	0.41
1:C:1226:VAL:HG11	1:C:1309:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:LYS:NZ	1:A:1214:ASP:O	2.52	0.41
1:C:1277:LEU:HD12	1:C:1277:LEU:O	2.21	0.41
1:A:1182:ALA:N	1:A:1230:GLN:HE21	2.18	0.40
2:F:158:SER:O	2:F:159:GLY:C	2.65	0.40
2:D:146:VAL:O	2:D:147:LEU:HB2	2.21	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	227/229 (99%)	219 (96%)	8 (4%)	0	100	100
1	C	223/229 (97%)	216 (97%)	7 (3%)	0	100	100
1	E	227/229 (99%)	219 (96%)	8 (4%)	0	100	100
2	B	260/285 (91%)	256 (98%)	4 (2%)	0	100	100
2	D	255/285 (90%)	251 (98%)	4 (2%)	0	100	100
2	F	256/285 (90%)	251 (98%)	5 (2%)	0	100	100
All	All	1448/1542 (94%)	1412 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/215 (99%)	209 (99%)	3 (1%)	59	82
1	C	206/215 (96%)	204 (99%)	2 (1%)	68	86
1	E	209/215 (97%)	204 (98%)	5 (2%)	43	72
2	B	229/249 (92%)	224 (98%)	5 (2%)	45	74
2	D	227/249 (91%)	224 (99%)	3 (1%)	61	83
2	F	223/249 (90%)	221 (99%)	2 (1%)	70	87
All	All	1306/1392 (94%)	1286 (98%)	20 (2%)	57	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1124	GLU
1	A	1242	VAL
1	A	1298	LYS
2	B	28	ARG
2	B	30	VAL
2	B	92	THR
2	B	134	GLN
2	B	216	LEU
1	C	1232	LEU
1	C	1308	ARG
2	D	55	ARG
2	D	171	ASN
2	D	204	ASN
1	E	1097	GLU
1	E	1113	GLN
1	E	1131	SER
1	E	1147	SER
1	E	1226	VAL
2	F	51	ILE
2	F	250	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1230	GLN
1	E	1113	GLN
1	E	1212	HIS
2	F	224	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 ⓘ

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	303	-	5,5,5	0.36	0	5,5,5	0.39	0
4	GOL	D	303	-	5,5,5	0.37	0	5,5,5	0.30	0
4	GOL	F	303	-	5,5,5	0.41	0	5,5,5	0.38	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
4	GOL	B	303	-	-	2/4/4/4	-
4	GOL	D	303	-	-	2/4/4/4	-
4	GOL	F	303	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	GOL	O1-C1-C2-O2
4	B	303	GOL	O1-C1-C2-C3
4	D	303	GOL	C1-C2-C3-O3
4	D	303	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	303	GOL	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 ⓘ

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	229/229 (100%)	0.46	5 (2%) 62 59	36, 53, 84, 100	0
1	C	225/229 (98%)	0.49	17 (7%) 20 17	38, 60, 126, 131	0
1	E	229/229 (100%)	0.15	8 (3%) 47 43	39, 62, 93, 122	0
2	B	264/285 (92%)	0.19	5 (1%) 66 63	32, 49, 78, 96	0
2	D	259/285 (90%)	0.33	8 (3%) 51 48	30, 63, 96, 115	0
2	F	260/285 (91%)	0.11	7 (2%) 56 53	33, 55, 92, 108	0
All	All	1466/1542 (95%)	0.28	50 (3%) 48 44	30, 57, 95, 131	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1182	ALA	5.0
1	C	1095	ILE	4.6
1	A	1101	PHE	4.1
2	F	263	GLY	4.0
1	E	1105	ASN	3.8
1	C	1101	PHE	3.6
1	E	1186	PHE	3.5
2	D	54	PHE	3.4
1	C	1099	ILE	3.3
2	F	204	ASN	3.2
1	A	1307	ASP	3.1
1	E	1183	ALA	3.1
1	C	1126	PHE	3.1
2	B	266	SER	3.1
1	C	1129	TRP	3.0
1	C	1093	GLU	3.0
2	F	274	GLY	3.0
2	F	203	LYS	2.9
1	C	1103	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	1098	LYS	2.8
1	A	1089	HIS	2.7
1	A	1317	SER	2.6
2	D	37	VAL	2.6
1	E	1101	PHE	2.6
2	B	203	LYS	2.5
1	A	1099	ILE	2.4
2	F	55	ARG	2.3
2	B	134	GLN	2.3
2	D	244	MET	2.3
2	F	244	MET	2.3
1	C	1102	ILE	2.2
2	D	274	GLY	2.2
1	C	1106	LEU	2.2
1	C	1306	LYS	2.2
1	C	1156	LEU	2.2
2	F	249	HIS	2.2
2	D	250	ILE	2.2
2	D	280	GLU	2.2
1	C	1121	THR	2.2
2	B	206	LYS	2.2
1	C	1115	VAL	2.2
1	C	1125	GLU	2.1
1	C	1118	LEU	2.1
1	E	1185	ASN	2.1
1	E	1089	HIS	2.1
2	B	245	PHE	2.1
2	D	253	ALA	2.0
2	D	206	LYS	2.0
1	C	1107	SER	2.0
1	E	1106	LEU	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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	F	303	6/6	0.81	0.23	44,55,71,71	0
4	GOL	D	303	6/6	0.91	0.12	51,64,70,77	0
4	GOL	B	303	6/6	0.92	0.14	44,53,57,59	0
5	CL	B	304	1/1	0.92	0.10	38,38,38,38	0
3	MG	D	301	1/1	0.96	0.06	55,55,55,55	0
3	MG	F	301	1/1	0.97	0.05	47,47,47,47	0
3	MG	B	305	1/1	0.98	0.04	63,63,63,63	0
3	MG	F	305	1/1	0.98	0.05	73,73,73,73	0
3	MG	D	302	1/1	0.98	0.04	55,55,55,55	0
5	CL	F	304	1/1	0.98	0.05	39,39,39,39	0
3	MG	B	301	1/1	0.99	0.04	36,36,36,36	0
3	MG	B	302	1/1	0.99	0.02	37,37,37,37	0
5	CL	D	304	1/1	0.99	0.05	44,44,44,44	0
3	MG	F	302	1/1	0.99	0.04	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.