



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 PM GMT

PDB ID : 4GMJ
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

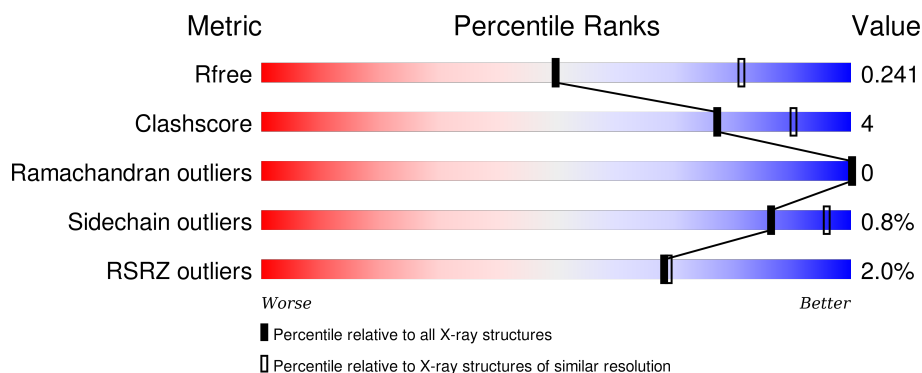
1 Overall quality at a glance ⓘ

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>88% 12%</div> </div>
1	C	229	<div> <div>2%</div> <div>89% 10% .</div> </div>
1	E	229	<div> <div>2%</div> <div>93% 7%</div> </div>
2	B	285	<div> <div>%</div> <div>82% 10% 7%</div> </div>
2	D	285	<div> <div>2%</div> <div>80% 11% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	285	 3% 85% 6% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	303	-	-	-	X
4	GOL	D	303	-	-	-	X
4	GOL	F	303	-	-	-	X

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

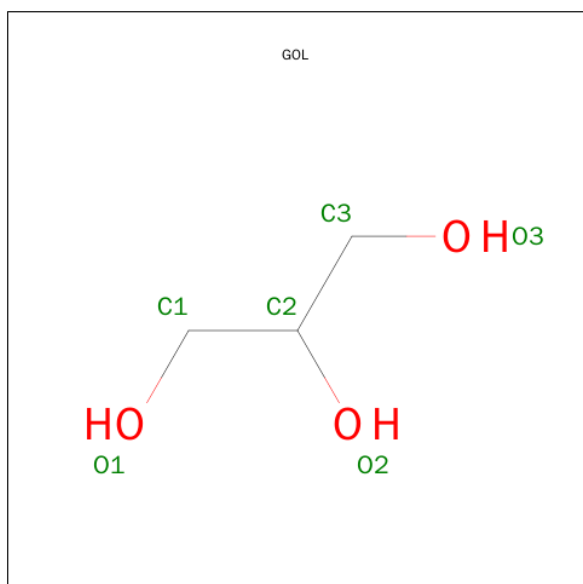
- Molecule 2 is a protein called CCR4-NOT transcription complex subunit 7.

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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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		

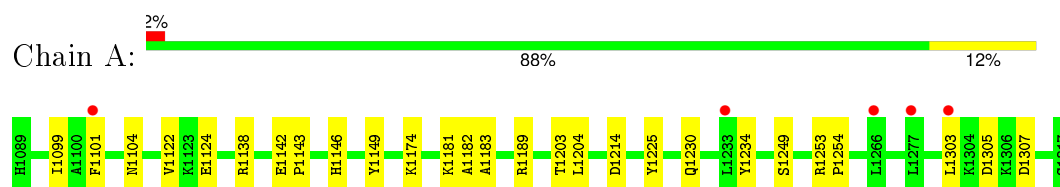
- Molecule 6 is water.

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

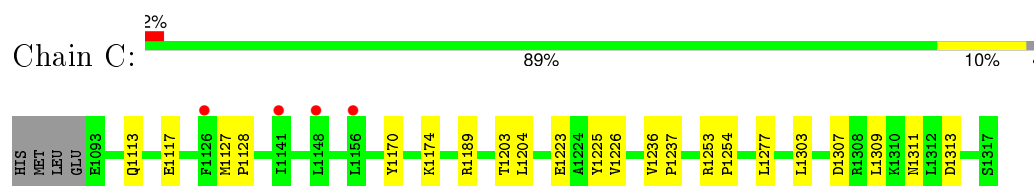
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

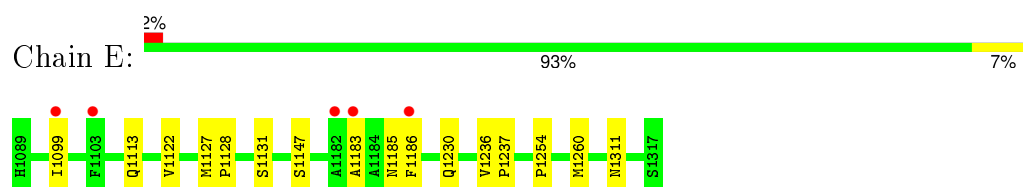
- Molecule 1: CCR4-NOT transcription complex subunit 1



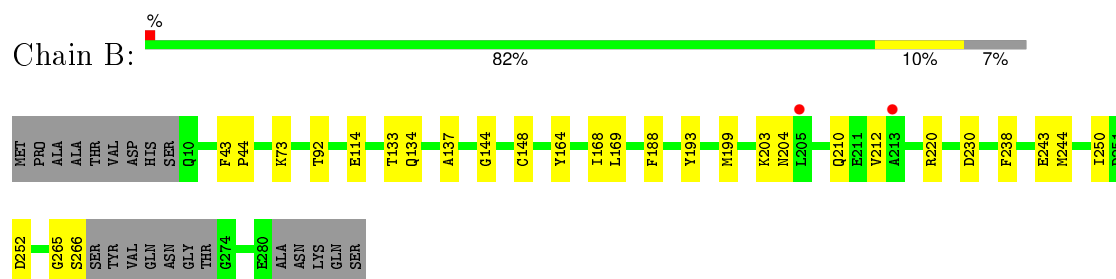
- Molecule 1: CCR4-NOT transcription complex subunit 1



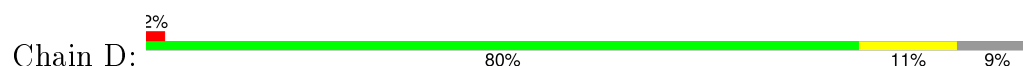
- Molecule 1: CCR4-NOT transcription complex subunit 1

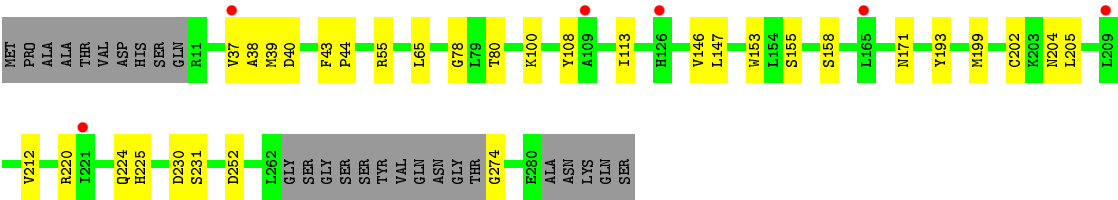


- Molecule 2: CCR4-NOT transcription complex subunit 7

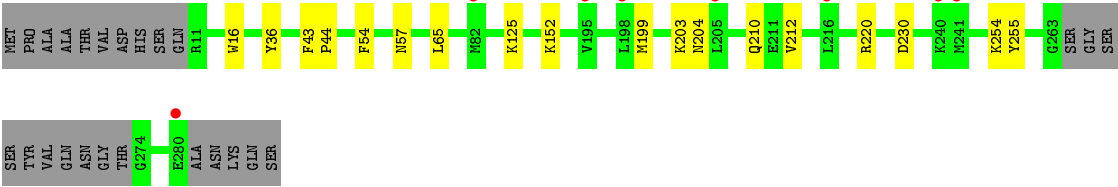
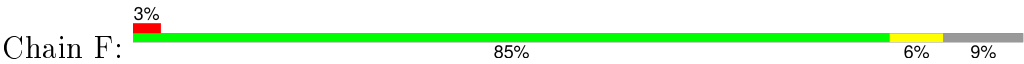


- Molecule 2: CCR4-NOT transcription complex subunit 7





• 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	82.47 Å 101.74 Å 142.20 Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	76.70 – 2.70 82.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (76.70-2.70) 95.2 (82.21-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.214 , 0.249 0.205 , 0.241	Depositor DCC
R_{free} test set	3059 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63192 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL

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	0.29	0/1894	0.48	0/2562
1	C	0.24	0/1850	0.40	0/2505
1	E	0.24	0/1883	0.40	0/2550
2	B	0.29	0/2185	0.47	0/2947
2	D	0.25	0/2160	0.41	0/2913
2	F	0.26	0/2145	0.42	0/2894
All	All	0.26	0/12117	0.43	0/16371

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	17	0
1	C	1816	1849	1844	15	0
1	E	1848	1879	1873	9	0
2	B	2137	2045	2040	16	0
2	D	2112	2027	2027	21	0
2	F	2097	2012	2007	11	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
6	E	19	0	0	0	0
6	F	49	0	0	0	0
All	All	12109	11741	11714	88	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 (88) 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
2:B:220:ARG:NH2	2:B:230:ASP:OD1	2.35	0.59
2:D:220:ARG:NH2	2:D:230:ASP:OD1	2.34	0.59
1:E:1099:ILE:HG22	1:E:1122:VAL:HG21	1.84	0.59
2:D:274:GLY:N	6:D:410:HOH:O	2.36	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
1:A:1181:LYS:C	1:A:1230:GLN:NE2	2.60	0.55
2:D:43:PHE:O	4:D:303:GOL:H32	2.08	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:GLU:OE2	1:C:1189:ARG:NH1	2.43	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
2:F:43:PHE:HB2	2:F:44:PRO:CD	2.40	0.51
1:A:1225:TYR:CG	1:A:1303:LEU:HD22	2.45	0.51
2:F:199:MET:SD	2:F:212:VAL:HG21	2.52	0.50
2:F:210:GLN:OE1	2:F:220:ARG:NH1	2.44	0.50
2:B:243:GLU:HG3	2:B:244:MET:N	2.26	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: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
2:F:65:LEU:HD23	2:F:65:LEU:C	2.35	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:A:1142:GLU:OE1	1:A:1149:TYR:OH	2.27	0.46
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
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: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
2:D:193:TYR:OH	2:D:252:ASP:OD1	2.25	0.45
2:D:100:LYS:NZ	6:D:426:HOH:O	2.50	0.45
2:D:65:LEU:HD23	2:D:65:LEU:C	2.37	0.45
1:C:1236:VAL:HB	1:C:1237:PRO:HD3	1.97	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:B:265:GLY:O	2:B:266:SER:C	2.55	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:D:220:ARG:HH12	2:D:224:GLN:HG3	1.83	0.44
2:B:137:ALA:HB2	2:B:168:ILE:HG22	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1127:MET:HA	1:C:1127:MET:HE2	2.01	0.43
1:E:1127:MET:N	1:E:1128:PRO:CD	2.81	0.43
1:A:1182:ALA:N	1:A:1230:GLN:NE2	2.67	0.43
1:C:1225:TYR:CG	1:C:1303:LEU:HD22	2.53	0.43
1:A:1225:TYR:CD2	1:A:1303:LEU:HD22	2.53	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
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:1254:PRO:HG3	1:E:1260:MET:HE1	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:A:1101:PHE:HA	1:A:1104:ASN:HB2	2.02	0.41
1:E:1185:ASN:O	1:E:1186:PHE:HB3	2.20	0.41
2:D:220:ARG:NH1	2:D:224:GLN:HG3	2.35	0.41
1:E:1311:ASN:N	1:E:1311:ASN:OD1	2.54	0.41
1:A:1253:ARG:O	1:A:1254:PRO:C	2.56	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
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: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 ⓘ

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%)	211 (100%)	1 (0%)	92	98
1	C	206/215 (96%)	205 (100%)	1 (0%)	92	98
1	E	209/215 (97%)	206 (99%)	3 (1%)	74	92
2	B	229/249 (92%)	227 (99%)	2 (1%)	84	95
2	D	227/249 (91%)	224 (99%)	3 (1%)	76	92
2	F	223/249 (90%)	223 (100%)	0	100	100
All	All	1306/1392 (94%)	1296 (99%)	10 (1%)	86	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1124	GLU
2	B	92	THR
2	B	134	GLN
1	C	1313	ASP
2	D	55	ARG
2	D	171	ASN
2	D	204	ASN

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Mol	Chain	Res	Type
1	E	1113	GLN
1	E	1131	SER
1	E	1147	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1230	GLN
2	B	76	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.33	0	5,5,5	0.36	0
4	GOL	D	303	-	5,5,5	0.35	0	5,5,5	0.19	0
4	GOL	F	303	-	5,5,5	0.38	0	5,5,5	0.33	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	-	-	0/4/4/4	0/0/0/0
4	GOL	D	303	-	-	0/4/4/4	0/0/0/0
4	GOL	F	303	-	-	0/4/4/4	0/0/0/0

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.

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%)	0.63	5 (2%) 65 66	33, 49, 76, 91	0
1	C	225/229 (98%)	0.52	4 (1%) 71 72	36, 54, 115, 122	0
1	E	229/229 (100%)	0.48	5 (2%) 65 66	35, 57, 87, 110	0
2	B	264/285 (92%)	0.54	2 (0%) 87 88	29, 45, 72, 89	0
2	D	259/285 (90%)	0.55	6 (2%) 64 64	30, 57, 89, 106	0
2	F	260/285 (91%)	0.48	8 (3%) 52 52	30, 50, 85, 101	0
All	All	1466/1542 (95%)	0.53	30 (2%) 68 69	29, 52, 88, 122	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1182	ALA	3.5
2	B	205	LEU	3.0
1	E	1183	ALA	2.9
2	F	280	GLU	2.7
1	C	1126	PHE	2.5
2	F	195	VAL	2.4
1	A	1277	LEU	2.4
2	F	198	LEU	2.3
2	F	205	LEU	2.3
1	E	1099	ILE	2.2
2	B	213	ALA	2.2
1	C	1156	LEU	2.2
1	E	1103	PHE	2.2
2	D	165	LEU	2.1
2	D	221	ILE	2.1
1	A	1233	LEU	2.1
2	D	126	HIS	2.1
2	D	109	ALA	2.1
1	A	1303	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1148	LEU	2.1
2	F	216	LEU	2.1
1	C	1141	ILE	2.1
2	D	37	VAL	2.1
1	E	1186	PHE	2.1
2	F	82	MET	2.1
2	D	209	LEU	2.0
1	A	1101	PHE	2.0
2	F	241	MET	2.0
1	A	1266	LEU	2.0
2	F	240	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	F	303	6/6	0.82	0.51	4.16	44,55,71,71	0
4	GOL	D	303	6/6	0.92	0.32	4.08	51,64,70,77	0
4	GOL	B	303	6/6	0.93	0.33	2.86	44,53,57,59	0
3	MG	D	301	1/1	0.83	0.15	-1.86	55,55,55,55	0
3	MG	B	302	1/1	0.98	0.16	-2.08	37,37,37,37	0
5	CL	D	304	1/1	0.98	0.14	-2.26	44,44,44,44	0
3	MG	D	302	1/1	0.84	0.14	-2.43	55,55,55,55	0
5	CL	B	304	1/1	0.91	0.17	-2.55	38,38,38,38	0
3	MG	F	302	1/1	0.97	0.13	-3.11	49,49,49,49	0
5	CL	F	304	1/1	0.97	0.13	-3.45	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	F	301	1/1	0.93	0.13	-	47,47,47,47	0
3	MG	F	305	1/1	0.86	0.06	-	73,73,73,73	0
3	MG	B	305	1/1	0.84	0.09	-	63,63,63,63	0
3	MG	B	301	1/1	0.96	0.17	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.