



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3UEZ
Title : Crystal structure of the human Colony-Stimulating Factor 1 (hCSF-1) cytokine
in complex with the viral receptor BARF1
Authors : Elegheert, J.; Bracke, N.; Savvides, S.N.
Deposited on : 2011-10-31
Resolution : 3.41 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

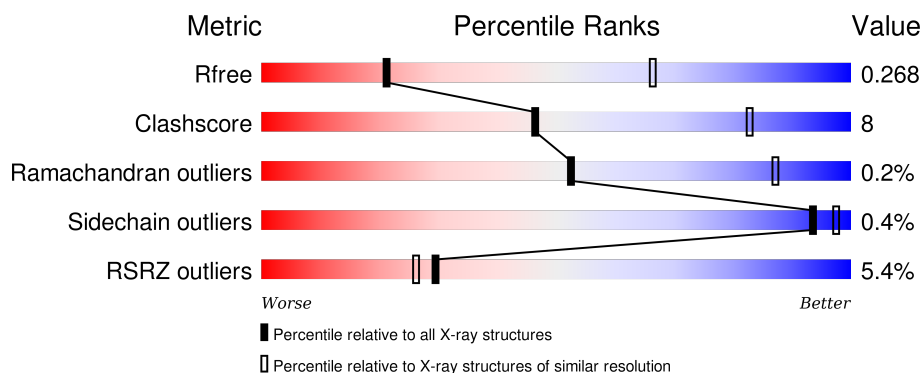
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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	208	<div> <div>77%</div> <div>12%</div> <div>11%</div> </div>
1	B	208	<div> <div>74%</div> <div>15%</div> <div>11%</div> </div>
1	C	208	<div> <div>70%</div> <div>20%</div> <div>11%</div> </div>
1	D	208	<div> <div>68%</div> <div>21%</div> <div>11%</div> </div>
2	E	153	<div> <div>7%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	153	
2	G	153	
2	H	153	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10693 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 Secreted protein BARF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1477	955	251	264	7			
1	B	185	Total	C	N	O	S	0	0	0
			1481	958	252	264	7			
1	C	186	Total	C	N	O	S	0	0	0
			1483	958	252	266	7			
1	D	186	Total	C	N	O	S	0	0	0
			1487	961	253	266	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	SER	THR	ENGINEERED MUTATION	UNP P03228
A	222	LYS	-	EXPRESSION TAG	UNP P03228
A	223	HIS	-	EXPRESSION TAG	UNP P03228
A	224	HIS	-	EXPRESSION TAG	UNP P03228
A	225	HIS	-	EXPRESSION TAG	UNP P03228
A	226	HIS	-	EXPRESSION TAG	UNP P03228
A	227	HIS	-	EXPRESSION TAG	UNP P03228
A	228	HIS	-	EXPRESSION TAG	UNP P03228
B	169	SER	THR	ENGINEERED MUTATION	UNP P03228
B	222	LYS	-	EXPRESSION TAG	UNP P03228
B	223	HIS	-	EXPRESSION TAG	UNP P03228
B	224	HIS	-	EXPRESSION TAG	UNP P03228
B	225	HIS	-	EXPRESSION TAG	UNP P03228
B	226	HIS	-	EXPRESSION TAG	UNP P03228
B	227	HIS	-	EXPRESSION TAG	UNP P03228
B	228	HIS	-	EXPRESSION TAG	UNP P03228
C	169	SER	THR	ENGINEERED MUTATION	UNP P03228
C	222	LYS	-	EXPRESSION TAG	UNP P03228
C	223	HIS	-	EXPRESSION TAG	UNP P03228
C	224	HIS	-	EXPRESSION TAG	UNP P03228
C	225	HIS	-	EXPRESSION TAG	UNP P03228

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Chain	Residue	Modelled	Actual	Comment	Reference
C	226	HIS	-	EXPRESSION TAG	UNP P03228
C	227	HIS	-	EXPRESSION TAG	UNP P03228
C	228	HIS	-	EXPRESSION TAG	UNP P03228
D	169	SER	THR	ENGINEERED MUTATION	UNP P03228
D	222	LYS	-	EXPRESSION TAG	UNP P03228
D	223	HIS	-	EXPRESSION TAG	UNP P03228
D	224	HIS	-	EXPRESSION TAG	UNP P03228
D	225	HIS	-	EXPRESSION TAG	UNP P03228
D	226	HIS	-	EXPRESSION TAG	UNP P03228
D	227	HIS	-	EXPRESSION TAG	UNP P03228
D	228	HIS	-	EXPRESSION TAG	UNP P03228

- Molecule 2 is a protein called Macrophage colony-stimulating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	142	Total	C	N	O	S	0	0	0
			1159	730	193	225	11			
2	F	141	Total	C	N	O	S	0	0	0
			1150	723	192	224	11			
2	G	143	Total	C	N	O	S	0	1	0
			1174	739	195	229	11			
2	H	139	Total	C	N	O	S	0	0	0
			1126	708	189	218	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P09603
E	-2	SER	-	EXPRESSION TAG	UNP P09603
E	-1	HIS	-	EXPRESSION TAG	UNP P09603
E	0	MET	-	EXPRESSION TAG	UNP P09603
F	-3	GLY	-	EXPRESSION TAG	UNP P09603
F	-2	SER	-	EXPRESSION TAG	UNP P09603
F	-1	HIS	-	EXPRESSION TAG	UNP P09603
F	0	MET	-	EXPRESSION TAG	UNP P09603
G	-3	GLY	-	EXPRESSION TAG	UNP P09603
G	-2	SER	-	EXPRESSION TAG	UNP P09603
G	-1	HIS	-	EXPRESSION TAG	UNP P09603
G	0	MET	-	EXPRESSION TAG	UNP P09603
H	-3	GLY	-	EXPRESSION TAG	UNP P09603
H	-2	SER	-	EXPRESSION TAG	UNP P09603
H	-1	HIS	-	EXPRESSION TAG	UNP P09603

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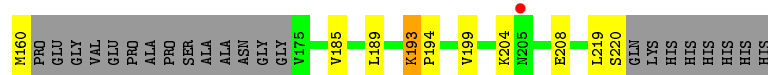
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	-	EXPRESSION TAG	UNP P09603

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

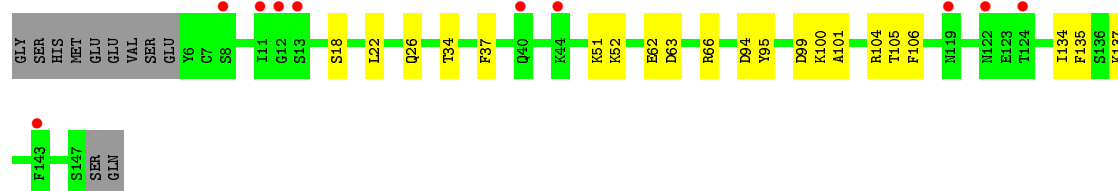
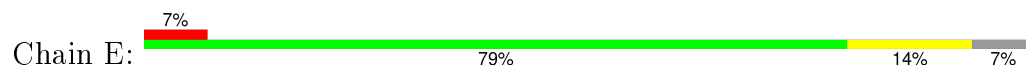
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	B	3	Total	C	N	O	0	0
			39	22	2	15		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 1: Secreted protein BARF1

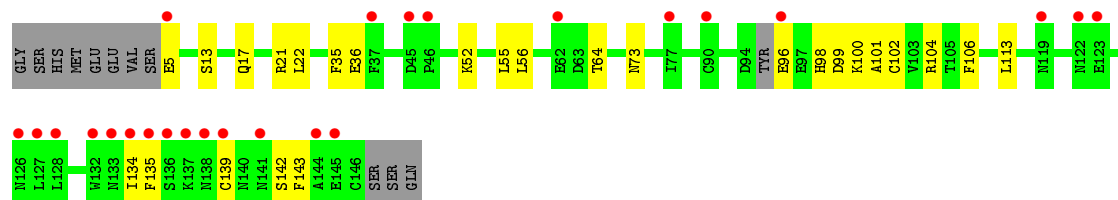
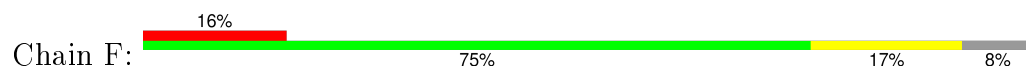




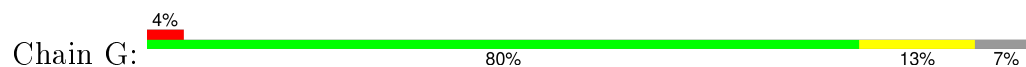
- Molecule 2: Macrophage colony-stimulating factor 1



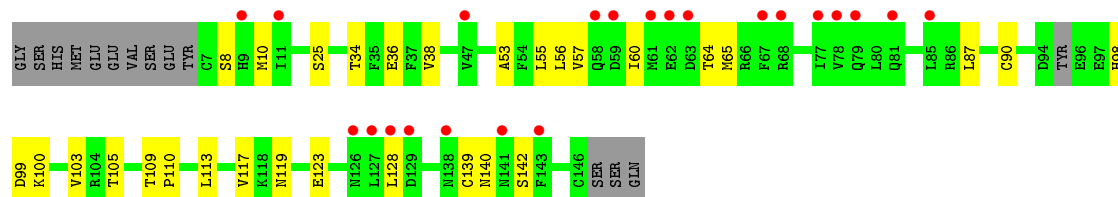
- Molecule 2: Macrophage colony-stimulating factor 1



- Molecule 2: Macrophage colony-stimulating factor 1



- Molecule 2: Macrophage colony-stimulating factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	235.24Å 235.24Å 95.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.41 58.81 – 3.41	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.00-3.41) 96.4 (58.81-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_874)	Depositor
R, R_{free}	0.231 , 0.274 0.219 , 0.268	Depositor DCC
R_{free} test set	1295 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 22.8	EDS
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 25861 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10693	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% 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: BMA, NAG

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	0.22	0/1520	0.41	0/2069
1	B	0.22	0/1524	0.41	0/2073
1	C	0.23	0/1526	0.41	0/2077
1	D	0.22	0/1530	0.40	0/2081
2	E	0.22	0/1179	0.36	0/1589
2	F	0.22	0/1168	0.37	0/1572
2	G	0.23	0/1197	0.36	0/1613
2	H	0.22	0/1143	0.37	0/1538
All	All	0.22	0/10787	0.39	0/14612

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	1477	0	1445	16	0
1	B	1481	0	1456	18	0
1	C	1483	0	1450	29	0
1	D	1487	0	1461	25	0
2	E	1159	0	1122	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1150	0	1113	20	0
2	G	1174	0	1136	17	0
2	H	1126	0	1094	26	0
3	A	39	0	34	1	0
3	B	39	0	34	0	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0
All	All	10693	0	10413	161	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 8.

All (161) 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:F:5:GLU:N	2:F:5:GLU:OE1	2.29	0.65
2:G:52:LYS:NZ	2:G:101:ALA:O	2.32	0.63
2:E:51:LYS:NZ	2:E:137:LYS:O	2.34	0.61
1:C:70:ILE:O	1:C:75:ARG:NH1	2.35	0.59
2:F:134:ILE:HG23	2:F:135:PHE:CD2	2.39	0.57
1:C:151:PHE:CG	1:C:152:PRO:HA	2.41	0.56
2:H:56:LEU:HD12	2:H:57:VAL:N	2.21	0.55
2:G:132:TRP:CZ3	2:G:133:ASN:HB2	2.42	0.55
2:E:34:THR:HG23	2:E:105:THR:CG2	2.36	0.55
2:G:5:GLU:HG3	2:G:132:TRP:CZ3	2.42	0.55
2:H:8:SER:HA	2:H:128:LEU:HD23	1.88	0.55
2:H:38:VAL:HG23	2:H:56:LEU:HD21	1.89	0.54
2:E:99:ASP:O	2:E:100:LYS:HB2	2.08	0.54
2:F:139:CYS:O	2:F:142:SER:N	2.40	0.54
1:B:193:LYS:HG3	1:B:194:PRO:HA	1.90	0.53
2:G:104:ARG:HD3	2:G:106:PHE:CZ	2.44	0.53
2:F:96:GLU:N	2:F:96:GLU:OE1	2.41	0.53
2:G:37:PHE:HB3	2:G:106:PHE:CE1	2.44	0.53
1:C:21:VAL:N	1:C:118:HIS:O	2.42	0.53
2:F:99:ASP:O	2:F:100:LYS:HB2	2.09	0.53
1:C:68:ILE:HD12	1:C:68:ILE:N	2.24	0.52
2:F:52:LYS:O	2:F:55:LEU:HG	2.08	0.52
1:D:193:LYS:HG3	1:D:194:PRO:HA	1.92	0.52
1:D:151:PHE:CG	1:D:152:PRO:HA	2.45	0.52
1:D:107:LYS:NZ	1:D:109:GLY:O	2.35	0.52
1:B:78:PHE:CE2	1:B:91:VAL:HG22	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HB2	1:A:208:GLU:O	2.10	0.52
2:H:55:LEU:HD12	2:H:56:LEU:N	2.24	0.52
1:A:151:PHE:CG	1:A:152:PRO:HA	2.45	0.51
1:B:94:ALA:HA	1:B:98:HIS:HD1	1.75	0.51
2:F:64:THR:HG21	2:F:113:LEU:HD21	1.92	0.51
1:B:68:ILE:N	1:B:68:ILE:HD12	2.26	0.50
2:F:104:ARG:HG3	2:F:106:PHE:CE1	2.45	0.50
1:A:72:TRP:N	1:A:73:PRO:CD	2.75	0.50
2:G:65:MET:HE2	2:G:117:VAL:HG21	1.94	0.50
2:H:8:SER:HA	2:H:128:LEU:CD2	2.42	0.50
2:F:64:THR:CG2	2:F:113:LEU:HD21	2.42	0.49
1:A:70:ILE:O	1:A:75:ARG:NH1	2.46	0.49
1:B:36:ARG:HG3	1:B:37:ARG:N	2.27	0.49
2:G:34:THR:CG2	2:G:105:THR:CG2	2.90	0.49
2:H:34:THR:HG23	2:H:105:THR:CG2	2.43	0.49
1:B:49:PHE:CD2	1:B:57:GLN:HG2	2.47	0.49
1:A:144:VAL:HG23	1:A:158:TRP:CZ2	2.48	0.49
1:D:72:TRP:N	1:D:73:PRO:CD	2.76	0.49
2:H:65:MET:CE	2:H:117:VAL:HG21	2.43	0.49
2:G:99:ASP:O	2:G:100:LYS:HB2	2.12	0.49
1:C:91:VAL:HG23	1:C:91:VAL:O	2.11	0.49
2:H:99:ASP:O	2:H:100:LYS:HB2	2.13	0.48
2:E:104:ARG:HG3	2:E:106:PHE:CE1	2.48	0.48
1:D:68:ILE:N	1:D:68:ILE:HD12	2.28	0.48
2:H:10:MET:HG2	2:H:87:LEU:CD2	2.43	0.48
1:B:72:TRP:N	1:B:73:PRO:CD	2.76	0.48
1:C:156:VAL:HG23	1:C:185:VAL:HG13	1.95	0.48
2:E:52:LYS:CE	2:E:101:ALA:O	2.62	0.48
1:C:34:TYR:CD1	2:H:34:THR:HG21	2.49	0.48
1:D:189:LEU:CD2	1:D:199:VAL:HG21	2.44	0.48
1:C:94:ALA:HA	1:C:98:HIS:HD1	1.79	0.48
2:G:65:MET:CE	2:G:117:VAL:HG21	2.43	0.48
1:A:94:ALA:HA	1:A:98:HIS:HD1	1.78	0.48
1:C:42:PRO:HG3	1:C:82:ARG:NH2	2.29	0.48
1:A:68:ILE:HD12	1:A:68:ILE:N	2.28	0.47
1:D:204:LYS:HB2	1:D:208:GLU:O	2.14	0.47
2:F:98:HIS:CG	2:F:143:PHE:HB3	2.50	0.47
1:C:23:ALA:CB	1:C:29:VAL:HG21	2.44	0.47
2:E:18:SER:O	2:E:22:LEU:HD13	2.15	0.47
2:G:5:GLU:HG3	2:G:132:TRP:CE3	2.49	0.47
2:F:101:ALA:O	2:F:102:CYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:PHE:CG	1:B:152:PRO:HA	2.49	0.47
1:C:96:ILE:HG23	1:C:151:PHE:CZ	2.49	0.46
2:H:64:THR:HG21	2:H:113:LEU:HD21	1.97	0.46
1:D:156:VAL:HG23	1:D:185:VAL:HG13	1.96	0.46
2:H:34:THR:CG2	2:H:105:THR:CG2	2.93	0.46
1:C:91:VAL:O	1:C:91:VAL:CG2	2.63	0.46
1:B:70:ILE:O	1:B:75:ARG:NH1	2.49	0.46
2:G:132:TRP:CE3	2:G:133:ASN:HB2	2.50	0.46
1:B:34:TYR:CD2	2:G:34:THR:HG21	2.51	0.46
2:E:94:ASP:O	2:E:95:TYR:CD1	2.69	0.46
1:D:70:ILE:O	1:D:75:ARG:NH1	2.49	0.46
1:C:144:VAL:HG23	1:C:158:TRP:CZ2	2.51	0.46
1:C:72:TRP:N	1:C:73:PRO:CD	2.79	0.45
2:H:65:MET:HE2	2:H:117:VAL:HG21	1.97	0.45
1:D:50:LYS:HD3	1:D:102:TYR:CE2	2.52	0.45
1:A:50:LYS:HG2	1:A:102:TYR:CE2	2.51	0.45
2:E:62:GLU:O	2:E:66:ARG:NH1	2.48	0.45
2:H:38:VAL:HG23	2:H:56:LEU:CD2	2.46	0.45
2:E:22:LEU:O	2:E:26:GLN:HG2	2.16	0.45
2:H:98:HIS:NE2	2:H:140:ASN:O	2.50	0.45
1:C:125:LEU:HD12	1:C:125:LEU:C	2.37	0.45
1:D:34:TYR:OH	2:F:36:GLU:HG3	2.16	0.45
1:C:189:LEU:CD2	1:C:199:VAL:HG21	2.47	0.45
2:E:104:ARG:HD3	2:E:106:PHE:CZ	2.52	0.44
2:E:134:ILE:HG23	2:E:135:PHE:N	2.31	0.44
2:H:36:GLU:HG2	2:H:103:VAL:CG2	2.47	0.44
2:F:17:GLN:O	2:F:21:ARG:HG3	2.17	0.44
2:F:13:SER:O	2:F:17:GLN:HG3	2.18	0.44
1:D:42:PRO:HG3	1:D:82:ARG:NH2	2.33	0.44
1:A:34:TYR:CD1	2:E:34:THR:HG21	2.53	0.44
2:F:35:PHE:CE1	2:F:106:PHE:HB2	2.53	0.44
1:A:23:ALA:CB	1:A:29:VAL:HG21	2.48	0.44
1:B:125:LEU:HD12	1:B:125:LEU:C	2.38	0.43
1:B:81:HIS:CE1	1:B:88:PHE:CD1	3.06	0.43
1:D:148:VAL:CG2	1:D:156:VAL:HG22	2.48	0.43
1:D:142:LEU:CD2	1:D:144:VAL:HG13	2.48	0.43
1:D:144:VAL:HG23	1:D:158:TRP:CZ2	2.53	0.43
1:D:127:LEU:HD23	1:D:127:LEU:C	2.39	0.43
1:B:142:LEU:HB2	1:B:195:TRP:CE2	2.53	0.43
1:C:127:LEU:HD23	1:C:127:LEU:C	2.39	0.43
1:C:151:PHE:CD2	1:C:152:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:ALA:O	2:H:57:VAL:HG23	2.18	0.43
1:A:148:VAL:CG2	1:A:156:VAL:HG22	2.49	0.43
2:H:36:GLU:O	2:H:60:ILE:HD11	2.19	0.43
2:H:64:THR:CG2	2:H:113:LEU:HD21	2.48	0.43
1:A:37:ARG:HG3	2:E:63:ASP:HB2	2.01	0.43
2:E:37:PHE:HB3	2:E:106:PHE:CE1	2.54	0.43
1:B:72:TRP:HA	1:B:75:ARG:HB2	2.01	0.42
1:C:78:PHE:CE2	1:C:91:VAL:HG12	2.54	0.42
1:D:136:PHE:CG	1:D:137:PRO:HA	2.55	0.42
2:H:36:GLU:HG2	2:H:103:VAL:HG21	2.02	0.42
2:G:10:MET:HG2	2:G:87:LEU:CD2	2.49	0.42
1:C:29:VAL:HB	1:C:91:VAL:HG22	2.02	0.42
2:G:25:SER:HB2	2:H:25:SER:OG	2.19	0.42
2:F:134:ILE:HG23	2:F:135:PHE:N	2.35	0.42
2:F:104:ARG:HD3	2:F:106:PHE:CZ	2.54	0.42
2:G:43:LEU:HG	2:G:146:CYS:SG	2.59	0.42
1:B:156:VAL:HG23	1:B:185:VAL:HG13	2.02	0.42
1:C:48:TRP:CE3	1:C:89:LEU:HD22	2.55	0.42
2:H:60:ILE:HG23	2:H:64:THR:OG1	2.20	0.41
1:A:23:ALA:CB	1:A:29:VAL:CG2	2.97	0.41
2:H:119:ASN:O	2:H:123:GLU:HG2	2.20	0.41
2:G:10:MET:HG2	2:G:87:LEU:HD23	2.02	0.41
1:C:48:TRP:CE2	1:C:89:LEU:HB2	2.55	0.41
1:D:219:LEU:O	1:D:220:SER:HB3	2.20	0.41
1:D:125:LEU:HD12	1:D:125:LEU:C	2.40	0.41
1:C:107:LYS:HE3	1:C:109:GLY:O	2.19	0.41
2:H:139:CYS:O	2:H:142:SER:N	2.53	0.41
1:C:136:PHE:CG	1:C:137:PRO:HA	2.55	0.41
1:D:29:VAL:HG12	1:D:91:VAL:HB	2.01	0.41
2:F:98:HIS:ND1	2:F:143:PHE:HB3	2.36	0.41
1:B:32:THR:HG22	1:B:88:PHE:CD2	2.56	0.41
2:F:22:LEU:HG	2:F:73:ASN:OD1	2.21	0.41
1:C:44:ILE:CG2	1:C:106:MET:HB2	2.49	0.41
1:B:130:HIS:CE1	1:B:145:THR:OG1	2.73	0.41
2:H:10:MET:HG3	2:H:87:LEU:HD21	2.03	0.41
1:C:123:LYS:NZ	1:C:180:ASP:OD2	2.44	0.41
1:A:127:LEU:C	1:A:127:LEU:HD23	2.40	0.41
3:A:301:NAG:H62	3:A:302:BMA:H2	2.03	0.41
2:G:101:ALA:O	2:G:102:CYS:HB2	2.20	0.41
1:C:143:THR:HG23	1:C:143:THR:O	2.21	0.41
1:C:23:ALA:CB	1:C:29:VAL:CG2	3.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:SER:O	1:D:84:ALA:HB3	2.20	0.41
1:D:159:LEU:O	1:D:160:MET:HB2	2.21	0.41
2:F:55:LEU:HD12	2:F:56:LEU:N	2.37	0.40
1:B:92:THR:HG23	1:B:93:ALA:N	2.36	0.40
1:D:96:ILE:HG23	1:D:151:PHE:CZ	2.56	0.40
1:D:48:TRP:CE2	1:D:89:LEU:HB2	2.57	0.40
1:C:148:VAL:HB	1:C:156:VAL:HG22	2.02	0.40
1:A:156:VAL:HG23	1:A:185:VAL:HG13	2.03	0.40
1:D:125:LEU:CB	1:D:150:ALA:HB2	2.51	0.40
2:H:109:THR:CG2	2:H:110:PRO:HD2	2.52	0.40
2:E:52:LYS:HE3	2:E:101:ALA:O	2.21	0.40
1:A:136:PHE:CG	1:A:137:PRO:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/208 (87%)	177 (98%)	4 (2%)	0	100	100
1	B	181/208 (87%)	173 (96%)	7 (4%)	1 (1%)	30	73
1	C	182/208 (88%)	178 (98%)	3 (2%)	1 (0%)	34	75
1	D	182/208 (88%)	174 (96%)	7 (4%)	1 (0%)	34	75
2	E	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	F	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
2	G	142/153 (93%)	139 (98%)	3 (2%)	0	100	100
2	H	135/153 (88%)	128 (95%)	7 (5%)	0	100	100
All	All	1280/1444 (89%)	1238 (97%)	39 (3%)	3 (0%)	52	87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	GLY
1	D	41	GLY
1	C	41	GLY

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	165/183 (90%)	165 (100%)	0	100	100
1	B	166/183 (91%)	165 (99%)	1 (1%)	90	96
1	C	166/183 (91%)	165 (99%)	1 (1%)	90	96
1	D	167/183 (91%)	165 (99%)	2 (1%)	78	91
2	E	134/145 (92%)	134 (100%)	0	100	100
2	F	133/145 (92%)	133 (100%)	0	100	100
2	G	136/145 (94%)	136 (100%)	0	100	100
2	H	130/145 (90%)	129 (99%)	1 (1%)	86	95
All	All	1197/1312 (91%)	1192 (100%)	5 (0%)	93	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	LYS
1	C	204	LYS
1	D	110	GLU
1	D	193	LYS
2	H	90	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	101	ASN
1	B	81	HIS

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Mol	Chain	Res	Type
1	B	118	HIS
1	B	130	HIS
1	C	57	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 ⓘ

12 carbohydrates 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	$\# Z > 2$
3	NAG	A	300	1,3	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
3	NAG	A	301	3	14,14,15	0.47	0	15,19,21	0.84	0
3	BMA	A	302	3	11,11,12	0.59	0	14,15,17	0.69	0
3	NAG	B	300	1,3	14,14,15	0.64	0	15,19,21	0.88	1 (6%)
3	NAG	B	301	3	14,14,15	0.47	0	15,19,21	0.66	0
3	BMA	B	302	3	11,11,12	0.58	0	14,15,17	0.76	0
3	NAG	C	300	1,3	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
3	NAG	C	301	3	14,14,15	0.48	0	15,19,21	0.67	0
3	BMA	C	302	3	11,11,12	0.56	0	14,15,17	0.76	0
3	NAG	D	300	1,3	14,14,15	0.61	0	15,19,21	1.06	1 (6%)
3	NAG	D	301	3	14,14,15	0.53	0	15,19,21	0.82	0
3	BMA	D	302	3	11,11,12	0.61	0	14,15,17	1.16	1 (7%)

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
3	NAG	A	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	301	3	-	0/6/23/26	0/1/1/1
3	BMA	A	302	3	-	0/2/19/22	0/1/1/1
3	NAG	B	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	301	3	-	0/6/23/26	0/1/1/1
3	BMA	B	302	3	-	0/2/19/22	0/1/1/1
3	NAG	C	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	301	3	-	0/6/23/26	0/1/1/1
3	BMA	C	302	3	-	0/2/19/22	0/1/1/1
3	NAG	D	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	301	3	-	0/6/23/26	0/1/1/1
3	BMA	D	302	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	NAG	C1-O5-C5	2.19	115.03	112.25
3	B	300	NAG	C4-C3-C2	2.38	114.94	111.23
3	D	300	NAG	C4-C3-C2	3.07	116.00	111.23
3	C	300	NAG	C1-O5-C5	3.33	116.47	112.25
3	D	302	BMA	C1-C2-C3	3.76	113.99	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAG	1	0
3	A	302	BMA	1	0

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	185/208 (88%)	0.23	2 (1%) 82 76	45, 60, 81, 94	0
1	B	185/208 (88%)	0.23	1 (0%) 91 89	46, 64, 80, 102	0
1	C	186/208 (89%)	0.15	3 (1%) 74 69	50, 63, 89, 108	0
1	D	186/208 (89%)	0.17	1 (0%) 91 89	45, 62, 85, 115	0
2	E	142/153 (92%)	0.43	10 (7%) 19 18	57, 85, 111, 119	0
2	F	141/153 (92%)	0.97	25 (17%) 2 2	61, 105, 153, 170	0
2	G	143/153 (93%)	0.29	6 (4%) 40 35	62, 90, 113, 138	0
2	H	139/153 (90%)	0.97	22 (15%) 3 3	56, 110, 148, 168	0
All	All	1307/1444 (90%)	0.40	70 (5%) 29 26	45, 72, 133, 170	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	133	ASN	8.0
2	H	79	GLN	6.5
2	H	138	ASN	5.5
2	F	136	SER	5.3
2	F	132	TRP	4.6
2	F	134	ILE	4.5
2	F	5	GLU	4.1
2	F	127	LEU	4.1
2	F	138	ASN	4.1
2	E	11	ILE	3.9
2	E	12	GLY	3.9
2	H	129	ASP	3.8
2	H	126	ASN	3.7
2	H	58	GLN	3.6
2	H	77	ILE	3.6
2	E	13	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	122	ASN	3.6
2	E	8	SER	3.5
1	C	220	SER	3.5
2	H	127	LEU	3.4
2	H	62	GLU	3.3
2	F	62	GLU	3.3
2	G	4	SER	3.3
2	F	135	PHE	3.3
2	G	132	TRP	3.2
2	F	123	GLU	3.2
2	F	46	PRO	3.2
2	F	96	GLU	3.1
2	F	145	GLU	3.1
2	H	67	PHE	3.1
2	F	126	ASN	2.9
2	H	63	ASP	2.9
2	H	59	ASP	2.7
2	E	40	GLN	2.7
2	E	122	ASN	2.7
2	F	119	ASN	2.7
1	C	61	GLY	2.7
2	E	124	THR	2.7
2	F	139	CYS	2.6
2	H	141	ASN	2.6
2	F	45	ASP	2.5
2	F	128	LEU	2.5
2	H	9	HIS	2.5
2	F	144	ALA	2.4
2	G	124	THR	2.4
2	F	137	LYS	2.4
2	H	11	ILE	2.4
2	H	78	VAL	2.4
2	H	61	MET	2.4
2	E	44	LYS	2.3
2	F	77	ILE	2.3
1	A	160	MET	2.2
2	G	142	SER	2.2
2	E	119	ASN	2.2
2	H	47	VAL	2.2
1	B	102	TYR	2.2
2	G	119	ASN	2.1
1	A	127	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	143	PHE	2.1
2	H	81	GLN	2.1
2	H	128	LEU	2.1
1	C	156	VAL	2.1
2	F	141	ASN	2.1
2	F	37	PHE	2.1
2	H	143	PHE	2.1
2	F	90	CYS	2.0
2	H	68	ARG	2.0
2	G	123	GLU	2.0
1	D	205	ASN	2.0
2	H	85	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](#)

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
3	NAG	C	300	14/15	0.94	0.16	-0.65	50,65,72,74	0
3	NAG	D	300	14/15	0.96	0.18	-0.66	50,62,66,68	0
3	NAG	A	300	14/15	0.93	0.19	-0.77	49,61,70,78	0
3	NAG	B	300	14/15	0.94	0.15	-1.82	42,60,63,69	0
3	NAG	A	301	14/15	0.92	0.23	-	63,70,80,81	0
3	BMA	D	302	11/12	0.82	0.20	-	70,80,91,97	0
3	BMA	A	302	11/12	0.84	0.17	-	74,80,89,91	0
3	BMA	C	302	11/12	0.82	0.18	-	71,80,88,93	0
3	BMA	B	302	11/12	0.69	0.37	-	67,75,94,96	0
3	NAG	B	301	14/15	0.91	0.22	-	60,64,70,71	0
3	NAG	D	301	14/15	0.95	0.14	-	52,64,80,85	0
3	NAG	C	301	14/15	0.93	0.16	-	61,68,72,73	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.