



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:41 AM UTC

PDB ID : 2P6S / pdb_00002p6s
Title : Crystal Structure of Transcriptional Regulator NMB0573/L-Met Complex from *Neisseria Meningitidis*
Authors : Ren, J.; Sainsbury, S.; Owens, R.J.; Oxford Protein Production Facility (OPPF)
Deposited on : 2007-03-19
Resolution : 2.80 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

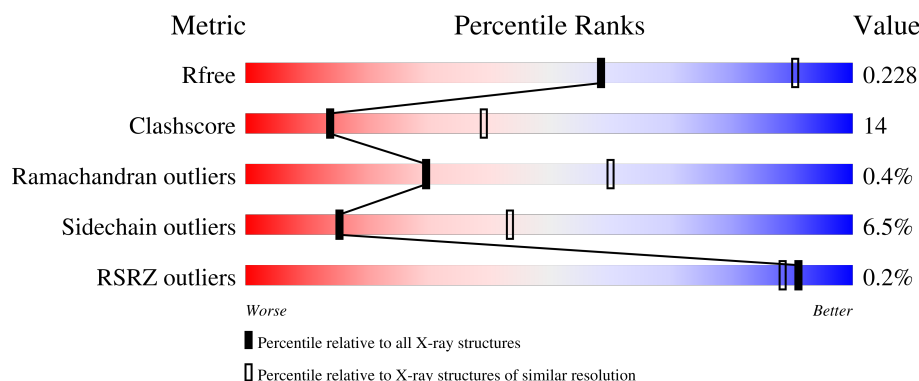
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	162	64% 30% • •
1	B	162	59% 32% 5% •
1	C	162	68% 25% • 5%
1	D	162	% 62% 31% • •
1	E	162	% 69% 27% • •

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Mol	Chain	Length	Quality of chain
1	F	162	 70%23%• 5%
1	G	162	 71%24%• •
1	H	162	 67%27%• 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10214 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 Transcriptional regulator, LRP/AsnC family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	0	0
			1235	786	216	230	2	1			
1	B	156	Total	C	N	O	S	Se	0	0	0
			1235	786	216	230	2	1			
1	C	154	Total	C	N	O	S	Se	0	0	0
			1218	775	213	227	2	1			
1	D	156	Total	C	N	O	S	Se	0	0	0
			1235	786	216	230	2	1			
1	E	156	Total	C	N	O	S	Se	0	0	0
			1235	786	216	230	2	1			
1	F	154	Total	C	N	O	S	Se	0	0	0
			1218	775	213	227	2	1			
1	G	158	Total	C	N	O	S	Se	0	0	0
			1250	796	218	232	2	2			
1	H	154	Total	C	N	O	S	Se	0	0	0
			1218	775	213	227	2	1			

There are 32 discrepancies between the modelled and reference sequences:

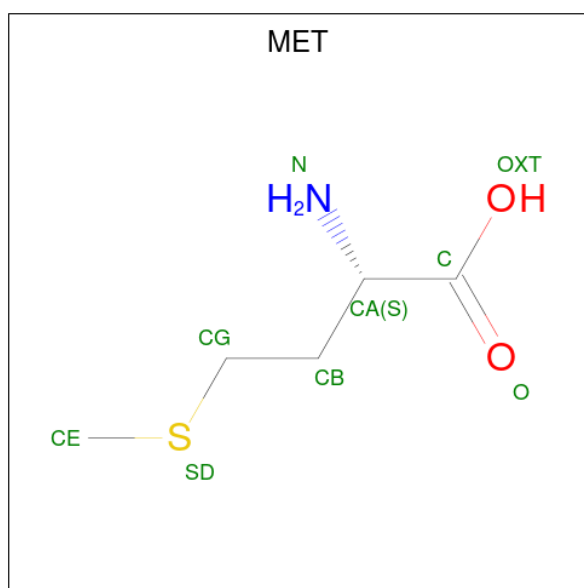
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q9K0L9
A	0	PRO	-	cloning artifact	UNP Q9K0L9
A	1	MSE	MET	modified residue	UNP Q9K0L9
A	117	MSE	MET	modified residue	UNP Q9K0L9
B	-1	GLY	-	cloning artifact	UNP Q9K0L9
B	0	PRO	-	cloning artifact	UNP Q9K0L9
B	1	MSE	MET	modified residue	UNP Q9K0L9
B	117	MSE	MET	modified residue	UNP Q9K0L9
C	-1	GLY	-	cloning artifact	UNP Q9K0L9
C	0	PRO	-	cloning artifact	UNP Q9K0L9
C	1	MSE	MET	modified residue	UNP Q9K0L9
C	117	MSE	MET	modified residue	UNP Q9K0L9
D	-1	GLY	-	cloning artifact	UNP Q9K0L9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	cloning artifact	UNP Q9K0L9
D	1	MSE	MET	modified residue	UNP Q9K0L9
D	117	MSE	MET	modified residue	UNP Q9K0L9
E	-1	GLY	-	cloning artifact	UNP Q9K0L9
E	0	PRO	-	cloning artifact	UNP Q9K0L9
E	1	MSE	MET	modified residue	UNP Q9K0L9
E	117	MSE	MET	modified residue	UNP Q9K0L9
F	-1	GLY	-	cloning artifact	UNP Q9K0L9
F	0	PRO	-	cloning artifact	UNP Q9K0L9
F	1	MSE	MET	modified residue	UNP Q9K0L9
F	117	MSE	MET	modified residue	UNP Q9K0L9
G	-1	GLY	-	cloning artifact	UNP Q9K0L9
G	0	PRO	-	cloning artifact	UNP Q9K0L9
G	1	MSE	MET	modified residue	UNP Q9K0L9
G	117	MSE	MET	modified residue	UNP Q9K0L9
H	-1	GLY	-	cloning artifact	UNP Q9K0L9
H	0	PRO	-	cloning artifact	UNP Q9K0L9
H	1	MSE	MET	modified residue	UNP Q9K0L9
H	117	MSE	MET	modified residue	UNP Q9K0L9

- Molecule 2 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	E	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	F	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	G	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
2	H	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Ca	0	0
			3	3		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	2	Total	Ca	0	0
			2	2		
4	F	2	Total	Ca	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	38	Total	O	0	0
			38	38		
5	C	25	Total	O	0	0
			25	25		
5	D	22	Total	O	0	0
			22	22		
5	E	25	Total	O	0	0
			25	25		

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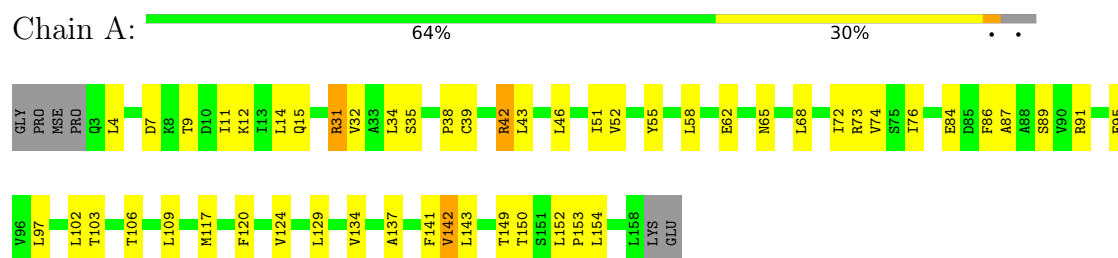
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	34	Total 34	O 34	0	0
5	G	19	Total 19	O 19	0	0
5	H	16	Total 16	O 16	0	0

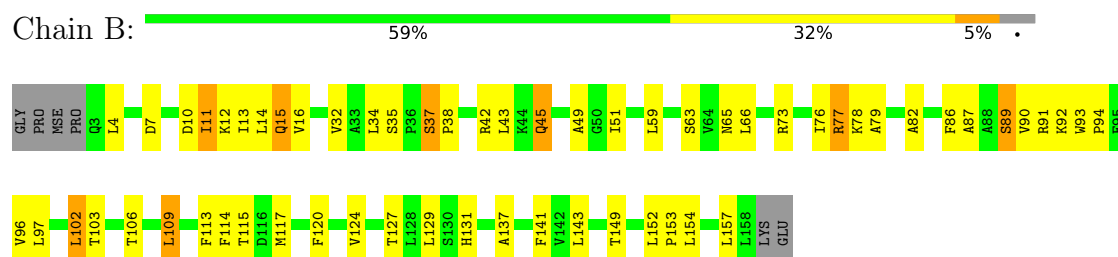
3 Residue-property plots [i](#)

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.

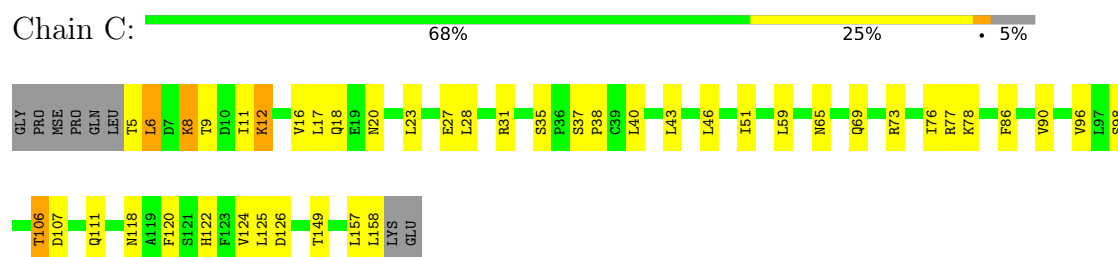
- Molecule 1: Transcriptional regulator, LRP/AsnC family



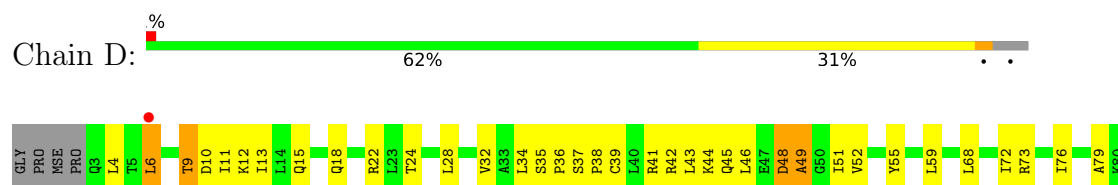
- Molecule 1: Transcriptional regulator, LRP/AsnC family

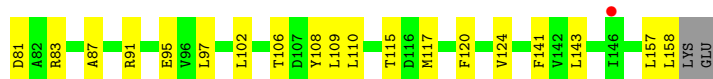


- Molecule 1: Transcriptional regulator, LRP/AsnC family



- Molecule 1: Transcriptional regulator, LRP/AsnC family





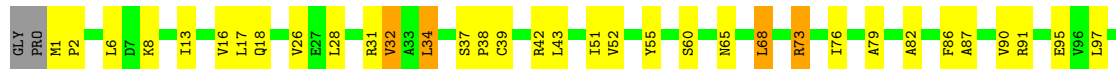
- Molecule 1: Transcriptional regulator, LRP/AsnC family



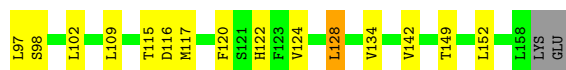
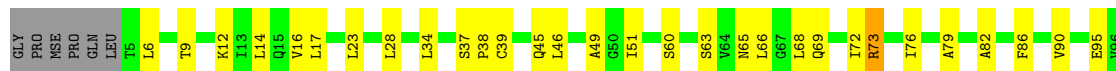
- Molecule 1: Transcriptional regulator, LRP/AsnC family



- Molecule 1: Transcriptional regulator, LRP/AsnC family



- Molecule 1: Transcriptional regulator, LRP/AsnC family



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.83Å 149.68Å 77.67Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.80) 99.8 (30.00-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.306 (Not available) , 0.228	Depositor DCC
R_{free} test set	1975 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10214	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.47% 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, CA

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	0.53	0/1255	0.75	0/1698
1	B	0.51	0/1255	0.75	0/1698
1	C	0.49	0/1238	0.74	0/1675
1	D	0.50	0/1255	0.74	0/1698
1	E	0.48	0/1255	0.73	0/1698
1	F	0.51	0/1238	0.74	0/1675
1	G	0.49	0/1271	0.72	0/1720
1	H	0.49	0/1238	0.76	0/1675
All	All	0.50	0/10005	0.74	0/13537

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

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	1235	0	1260	50	0
1	B	1235	0	1260	57	0
1	C	1218	0	1241	33	0
1	D	1235	0	1260	52	0
1	E	1235	0	1260	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1218	0	1241	36	0
1	G	1250	0	1279	36	0
1	H	1218	0	1241	38	0
2	A	9	0	8	0	0
2	B	9	0	8	0	0
2	C	9	0	8	1	0
2	D	9	0	8	0	0
2	E	9	0	8	0	0
2	F	9	0	8	1	0
2	G	9	0	8	1	0
2	H	9	0	8	0	0
3	A	36	0	48	1	0
3	C	12	0	16	0	0
3	E	6	0	8	0	0
3	F	12	0	16	0	0
3	H	6	0	8	3	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	38	0	0	0	0
5	B	38	0	0	1	0
5	C	25	0	0	0	0
5	D	22	0	0	2	0
5	E	25	0	0	0	0
5	F	34	0	0	0	0
5	G	19	0	0	1	0
5	H	16	0	0	0	0
All	All	10214	0	10202	291	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 14.

All (291) 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:A:42:ARG:HG2	1:A:42:ARG:HH21	1.09	1.18
1:A:68:LEU:HD21	1:A:117:MSE:HE2	1.23	1.16
1:D:120:PHE:O	1:D:124:VAL:HG23	1.68	0.93
1:A:124:VAL:HG11	1:D:143:LEU:CD2	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HG2	1:A:42:ARG:NH2	1.84	0.91
1:A:42:ARG:HH21	1:A:42:ARG:CG	1.84	0.90
1:A:141:PHE:HB2	1:D:117:MSE:HE2	1.52	0.90
1:C:59:LEU:HD22	1:D:51:ILE:HG22	1.59	0.84
1:A:68:LEU:HD21	1:A:117:MSE:CE	2.05	0.84
1:E:97:LEU:HD21	1:F:152:LEU:HD23	1.59	0.82
1:C:59:LEU:HD12	1:D:18:GLN:NE2	1.96	0.80
1:D:120:PHE:CE2	1:D:124:VAL:HG21	2.17	0.80
1:G:152:LEU:HD23	1:H:97:LEU:HD21	1.62	0.80
1:B:10:ASP:O	1:B:14:LEU:HD12	1.81	0.79
1:F:46:LEU:HD23	1:F:51:ILE:HD12	1.65	0.78
1:A:11:ILE:HA	1:A:14:LEU:HD12	1.65	0.77
1:G:17:LEU:HD21	1:G:28:LEU:HD22	1.64	0.77
1:A:73:ARG:HD2	1:A:106:THR:HG21	1.67	0.77
1:C:69:GLN:HE21	1:C:111:GLN:HE21	1.31	0.75
1:D:68:LEU:HD11	1:D:141:PHE:CD1	2.24	0.73
1:C:11:ILE:HD12	1:C:158:LEU:CD2	2.18	0.73
1:A:117:MSE:HG3	1:D:68:LEU:HD13	1.70	0.72
1:A:124:VAL:HG11	1:D:143:LEU:HD22	1.69	0.72
1:E:17:LEU:HD21	1:E:28:LEU:HD22	1.71	0.72
1:B:11:ILE:HD11	1:B:157:LEU:HB2	1.71	0.71
1:C:76:ILE:HD11	1:C:86:PHE:CG	2.26	0.71
1:H:14:LEU:HD11	1:H:51:ILE:HG21	1.73	0.70
1:A:143:LEU:HD23	1:D:117:MSE:HE3	1.73	0.70
1:G:79:ALA:HB3	1:G:82:ALA:HB2	1.73	0.70
1:G:13:ILE:HD13	1:G:32:VAL:HG21	1.74	0.69
1:A:152:LEU:HD23	1:B:97:LEU:HD21	1.75	0.69
1:B:12:LYS:O	1:B:16:VAL:HG23	1.91	0.68
1:A:68:LEU:CD2	1:A:117:MSE:HE2	2.14	0.68
1:B:13:ILE:HD11	1:B:32:VAL:HG21	1.75	0.68
1:F:58:LEU:HD11	1:F:150:THR:HG21	1.75	0.66
1:C:11:ILE:HD12	1:C:158:LEU:HD23	1.75	0.66
1:C:46:LEU:HD22	1:C:51:ILE:HD12	1.78	0.66
1:C:149:THR:HG22	1:D:97:LEU:O	1.96	0.66
1:A:87:ALA:HB1	1:A:91:ARG:HH12	1.61	0.65
1:A:129:LEU:HD21	1:A:137:ALA:HB3	1.77	0.65
1:A:117:MSE:HE1	1:A:141:PHE:CE1	2.32	0.65
1:C:46:LEU:CD2	1:C:51:ILE:HD12	2.27	0.64
1:H:79:ALA:HB3	1:H:82:ALA:HB2	1.79	0.64
1:B:97:LEU:HD11	1:B:113:PHE:HD2	1.63	0.64
1:B:79:ALA:HB3	1:B:82:ALA:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:PHE:CE2	1:E:124:VAL:HG21	2.33	0.63
1:G:152:LEU:HD13	1:H:66:LEU:HD12	1.80	0.63
1:C:125:LEU:HD23	1:E:83:ARG:NH2	2.13	0.63
1:E:139:SER:O	1:G:103:THR:CG2	2.47	0.63
1:A:117:MSE:HE1	1:A:141:PHE:CZ	2.33	0.63
1:B:129:LEU:HD21	1:B:137:ALA:CB	2.29	0.62
1:G:16:VAL:HG11	1:G:31:ARG:HG2	1.80	0.62
1:B:15:GLN:HE21	1:B:15:GLN:HA	1.64	0.62
1:E:115:THR:CG2	1:F:156:HIS:ND1	2.62	0.62
1:H:76:ILE:HD11	1:H:86:PHE:CG	2.34	0.62
1:B:117:MSE:HE3	1:G:68:LEU:HD21	1.81	0.61
1:B:4:LEU:HD11	1:B:49:ALA:HB2	1.83	0.61
1:C:90:VAL:HG13	1:C:96:VAL:HG11	1.81	0.61
1:E:73:ARG:HG2	1:E:106:THR:HG21	1.81	0.61
1:F:124:VAL:HG12	1:F:125:LEU:HD12	1.83	0.60
1:D:9:THR:HG22	1:D:12:LYS:HD3	1.82	0.60
1:F:90:VAL:HG22	1:F:96:VAL:HG11	1.82	0.60
1:A:97:LEU:O	1:B:149:THR:HG22	2.01	0.60
1:A:103:THR:HG22	1:B:143:LEU:HD11	1.84	0.60
1:H:12:LYS:O	1:H:16:VAL:HG23	2.02	0.59
1:B:13:ILE:HD13	1:B:32:VAL:HG11	1.83	0.59
1:F:76:ILE:HD11	1:F:86:PHE:CD2	2.36	0.59
1:F:23:LEU:HD22	1:F:27:GLU:HG3	1.84	0.59
1:E:96:VAL:HG22	1:E:112:ALA:HB2	1.85	0.59
1:G:97:LEU:HD21	1:H:152:LEU:HD23	1.84	0.59
1:H:102:LEU:HD11	1:H:109:LEU:HD22	1.84	0.59
1:A:43:LEU:HA	1:A:46:LEU:HD12	1.84	0.59
1:A:149:THR:HG22	1:B:97:LEU:O	2.03	0.59
1:D:87:ALA:HB1	1:D:91:ARG:NH1	2.18	0.58
1:F:90:VAL:CG2	1:F:96:VAL:HG11	2.33	0.58
1:A:129:LEU:HD21	1:A:137:ALA:CB	2.33	0.58
1:B:97:LEU:CD1	1:B:113:PHE:HD2	2.16	0.58
1:A:97:LEU:HD21	1:B:152:LEU:HD23	1.84	0.58
1:B:102:LEU:HD22	1:B:109:LEU:HB2	1.86	0.58
1:A:51:ILE:HD13	1:B:63:SER:HB2	1.85	0.58
1:D:34:LEU:HD23	1:D:35:SER:N	2.18	0.58
1:E:12:LYS:O	1:E:16:VAL:HG23	2.04	0.58
1:H:68:LEU:HD23	3:H:809:GOL:H12	1.85	0.58
1:E:13:ILE:CG1	1:E:32:VAL:HG11	2.34	0.57
1:B:4:LEU:HD21	1:B:45:GLN:HG2	1.86	0.57
1:B:14:LEU:HD21	1:B:51:ILE:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:ASP:HA	3:H:809:GOL:H11	1.86	0.57
1:C:11:ILE:HD12	1:C:158:LEU:HD21	1.85	0.57
1:D:158:LEU:HD12	1:D:158:LEU:O	2.04	0.57
1:E:28:LEU:CD2	1:E:43:LEU:HD22	2.35	0.57
1:E:97:LEU:O	1:F:149:THR:HG22	2.05	0.57
1:F:87:ALA:O	1:F:90:VAL:HG12	2.05	0.57
1:B:11:ILE:CD1	1:B:157:LEU:HB2	2.36	0.56
1:F:46:LEU:CD2	1:F:51:ILE:HD12	2.35	0.56
1:E:152:LEU:HD23	1:F:97:LEU:HD21	1.87	0.56
1:E:102:LEU:HD23	1:F:142:VAL:HA	1.88	0.56
1:F:83:ARG:NH1	2:F:1160:MET:HE2	2.21	0.56
1:A:102:LEU:HD11	1:A:109:LEU:HD22	1.87	0.55
1:D:73:ARG:HB3	1:D:106:THR:HG21	1.88	0.55
1:F:37:SER:HB3	1:F:38:PRO:HD3	1.89	0.55
1:B:87:ALA:O	1:B:91:ARG:HG3	2.06	0.55
1:D:120:PHE:CZ	1:D:124:VAL:HG21	2.42	0.55
1:C:23:LEU:HD11	1:C:31:ARG:CZ	2.36	0.55
1:C:43:LEU:HD21	1:D:22:ARG:HH12	1.71	0.55
1:D:12:LYS:HB3	1:D:32:VAL:HG12	1.88	0.55
1:F:76:ILE:HG23	1:F:133:GLY:O	2.07	0.55
1:H:128:LEU:CD1	1:H:134:VAL:HG11	2.36	0.54
1:G:120:PHE:CZ	1:G:124:VAL:HG21	2.43	0.54
1:A:143:LEU:CD2	1:D:117:MSE:HE3	2.37	0.54
1:D:72:ILE:HD11	1:D:120:PHE:HE1	1.72	0.54
1:B:14:LEU:CD2	1:B:51:ILE:HG21	2.38	0.54
1:C:86:PHE:O	1:C:90:VAL:HG23	2.07	0.54
1:E:97:LEU:HD12	1:E:97:LEU:N	2.22	0.54
1:E:74:VAL:CG2	1:E:110:LEU:HD13	2.38	0.54
1:C:12:LYS:O	1:C:16:VAL:HG23	2.08	0.54
1:C:8:LYS:HE3	1:C:158:LEU:HD22	1.89	0.53
1:H:60:SER:O	1:H:63:SER:OG	2.20	0.53
1:F:87:ALA:HB1	1:F:91:ARG:NH1	2.23	0.53
1:C:17:LEU:HD21	1:C:28:LEU:HD22	1.89	0.53
1:G:26:VAL:HG13	5:G:1167:HOH:O	2.08	0.53
1:H:69:GLN:O	1:H:142:VAL:HG12	2.09	0.53
1:D:46:LEU:HD22	1:D:51:ILE:HD12	1.90	0.53
1:F:58:LEU:HD11	1:F:150:THR:CG2	2.39	0.53
1:B:129:LEU:HD21	1:B:137:ALA:HB3	1.90	0.53
1:B:15:GLN:HG2	1:B:154:LEU:HD12	1.90	0.52
1:E:59:LEU:HD22	1:F:51:ILE:HG22	1.91	0.52
1:F:24:THR:HG23	1:F:27:GLU:OE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD23	1:A:4:LEU:H	1.73	0.52
1:D:6:LEU:HD11	1:D:157:LEU:HD13	1.90	0.52
1:A:124:VAL:CG1	1:D:143:LEU:CD2	2.83	0.52
1:H:9:THR:HG21	1:H:34:LEU:HD11	1.91	0.52
1:H:128:LEU:C	1:H:128:LEU:HD13	2.34	0.52
1:H:79:ALA:HB3	1:H:82:ALA:CB	2.40	0.51
1:B:35:SER:O	1:B:38:PRO:HD2	2.10	0.51
1:H:69:GLN:HB3	1:H:142:VAL:CG1	2.39	0.51
1:E:124:VAL:HG12	1:E:129:LEU:HD12	1.92	0.51
1:D:24:THR:HA	5:D:1163:HOH:O	2.09	0.51
1:E:13:ILE:HG12	1:E:32:VAL:HG11	1.91	0.51
1:H:9:THR:CG2	1:H:34:LEU:HD11	2.41	0.51
1:B:7:ASP:OD2	1:B:7:ASP:C	2.53	0.51
1:D:34:LEU:HD11	1:D:42:ARG:HG3	1.93	0.51
1:D:44:LYS:O	1:D:48:ASP:HB2	2.10	0.51
1:E:139:SER:OG	2:G:1160:MET:OXT	2.27	0.51
1:D:79:ALA:HB3	5:D:1178:HOH:O	2.11	0.50
1:B:76:ILE:HD11	1:B:86:PHE:CD2	2.46	0.50
1:A:124:VAL:CG1	1:D:143:LEU:HD22	2.39	0.50
1:B:13:ILE:CD1	1:B:32:VAL:HG21	2.42	0.50
1:G:86:PHE:O	1:G:90:VAL:HG23	2.11	0.50
1:H:17:LEU:HD21	1:H:28:LEU:HD22	1.93	0.50
1:B:89:SER:OG	1:B:131:HIS:NE2	2.45	0.50
1:D:52:VAL:HG11	1:D:55:TYR:CZ	2.47	0.50
1:A:142:VAL:HG12	1:B:102:LEU:HD11	1.93	0.50
1:B:129:LEU:HD21	1:B:137:ALA:HB2	1.92	0.49
1:B:102:LEU:HD22	1:B:109:LEU:CB	2.42	0.49
1:C:23:LEU:HD22	1:C:27:GLU:CB	2.42	0.49
1:G:87:ALA:HB1	1:G:91:ARG:HH21	1.78	0.49
1:D:32:VAL:HG23	1:D:34:LEU:HB2	1.95	0.49
1:F:68:LEU:HD11	1:F:141:PHE:CD1	2.48	0.49
1:G:34:LEU:HD11	1:G:42:ARG:HD2	1.93	0.49
1:A:52:VAL:HG22	1:B:59:LEU:CD2	2.43	0.49
1:E:149:THR:HG22	1:F:97:LEU:O	2.12	0.49
1:A:95:GLU:HA	1:B:153:PRO:HG3	1.95	0.48
1:G:43:LEU:HD11	1:G:55:TYR:OH	2.13	0.48
1:A:9:THR:HG21	1:A:34:LEU:HG	1.96	0.48
1:H:72:ILE:HD11	1:H:120:PHE:HE1	1.79	0.48
1:C:8:LYS:NZ	1:C:158:LEU:HD13	2.29	0.48
1:B:103:THR:HG21	1:D:117:MSE:HE1	1.96	0.48
1:B:124:VAL:HG21	1:G:143:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:HB3	1:A:106:THR:HG21	1.95	0.48
1:B:11:ILE:HA	1:B:14:LEU:HD12	1.95	0.47
1:D:10:ASP:HA	1:D:13:ILE:HD12	1.95	0.47
1:F:58:LEU:CD1	1:F:150:THR:HG21	2.43	0.47
1:F:6:LEU:HD22	1:F:46:LEU:HD21	1.95	0.47
1:G:37:SER:HB3	1:G:38:PRO:HD3	1.95	0.47
1:G:149:THR:HG22	1:H:97:LEU:O	2.14	0.47
1:C:6:LEU:HD23	1:C:157:LEU:HD13	1.96	0.47
1:D:43:LEU:HD11	1:D:55:TYR:OH	2.14	0.47
1:E:4:LEU:HD21	1:E:45:GLN:NE2	2.30	0.47
1:E:42:ARG:O	1:E:45:GLN:HG2	2.13	0.47
1:A:58:LEU:HD11	1:A:150:THR:HG21	1.96	0.47
1:C:35:SER:O	1:C:38:PRO:HD2	2.15	0.47
1:E:49:ALA:HB3	1:E:51:ILE:HD13	1.96	0.47
1:H:76:ILE:CG2	1:H:82:ALA:HB1	2.44	0.47
1:D:41:ARG:O	1:D:44:LYS:HB3	2.15	0.47
1:A:153:PRO:O	1:B:66:LEU:HD11	2.15	0.46
1:C:59:LEU:CD2	1:D:51:ILE:HG22	2.40	0.46
1:G:76:ILE:HD11	1:G:86:PHE:CG	2.50	0.46
1:A:35:SER:O	1:A:38:PRO:HD2	2.15	0.46
1:C:59:LEU:HD23	1:D:52:VAL:HA	1.96	0.46
1:C:122:HIS:ND1	1:C:126:ASP:OD2	2.47	0.46
1:D:120:PHE:CZ	1:D:124:VAL:CG2	2.98	0.46
1:C:76:ILE:HG22	1:C:77:ARG:O	2.15	0.46
1:B:120:PHE:O	1:B:124:VAL:HG22	2.15	0.46
1:A:76:ILE:HD11	1:A:86:PHE:CG	2.50	0.46
1:B:141:PHE:CG	1:G:117:MSE:HE3	2.50	0.46
1:D:102:LEU:HD11	1:D:109:LEU:HD22	1.96	0.46
1:E:4:LEU:HD21	1:E:45:GLN:CD	2.41	0.46
1:H:73:ARG:CZ	1:H:109:LEU:HD13	2.45	0.46
1:E:74:VAL:HG23	1:E:110:LEU:HD13	1.98	0.46
1:F:87:ALA:HB1	1:F:91:ARG:HH12	1.80	0.46
1:D:83:ARG:HG3	1:D:108:TYR:OH	2.16	0.45
1:E:22:ARG:HD2	1:F:21:GLY:O	2.15	0.45
1:E:13:ILE:HG23	1:E:28:LEU:HD21	1.98	0.45
1:G:1:MSE:N	1:G:1:MSE:HE2	2.32	0.45
1:D:109:LEU:C	1:D:110:LEU:HD12	2.41	0.45
1:E:49:ALA:CB	1:E:51:ILE:HD13	2.47	0.45
1:E:129:LEU:HD21	1:E:137:ALA:HB3	1.97	0.45
1:C:69:GLN:HE21	1:C:111:GLN:NE2	2.05	0.45
1:E:129:LEU:HD21	1:E:137:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:VAL:HG11	1:G:55:TYR:CZ	2.52	0.45
1:G:73:ARG:HH12	1:H:73:ARG:NH2	2.14	0.45
1:G:6:LEU:HD21	1:G:51:ILE:HD11	1.98	0.45
1:B:73:ARG:CD	1:B:106:THR:HG21	2.47	0.45
1:B:93:TRP:CZ2	1:B:127:THR:HG22	2.52	0.45
1:D:28:LEU:O	1:D:32:VAL:HG22	2.17	0.45
1:G:2:PRO:HG3	1:H:65:ASN:HD22	1.81	0.45
1:H:69:GLN:HB3	1:H:142:VAL:HG11	1.98	0.45
1:B:114:PHE:CE2	1:B:120:PHE:HD1	2.33	0.45
1:E:43:LEU:HD11	1:E:55:TYR:OH	2.17	0.44
1:E:115:THR:HG23	1:F:156:HIS:ND1	2.31	0.44
1:G:120:PHE:CE2	1:G:124:VAL:HG21	2.53	0.44
1:H:128:LEU:CD1	1:H:128:LEU:C	2.91	0.44
1:B:4:LEU:HD22	1:B:42:ARG:NH1	2.32	0.44
1:E:24:THR:HG23	1:E:27:GLU:H	1.82	0.44
1:E:139:SER:O	1:G:103:THR:HG21	2.18	0.44
1:F:76:ILE:HD11	1:F:86:PHE:CG	2.52	0.44
1:A:15:GLN:HG2	1:A:154:LEU:HD12	2.00	0.44
1:D:34:LEU:HD23	1:D:35:SER:H	1.83	0.44
1:F:120:PHE:CE2	1:F:124:VAL:HG21	2.53	0.44
1:H:46:LEU:HD23	1:H:51:ILE:HD12	1.99	0.44
1:A:73:ARG:CD	1:A:106:THR:HG21	2.43	0.44
1:F:13:ILE:CG1	1:F:32:VAL:HG11	2.48	0.44
1:H:120:PHE:O	1:H:124:VAL:HG12	2.18	0.43
1:D:48:ASP:OD2	1:D:48:ASP:N	2.50	0.43
1:E:51:ILE:N	1:E:51:ILE:CD1	2.81	0.43
1:H:37:SER:N	1:H:38:PRO:HD2	2.34	0.43
1:B:37:SER:HB2	1:B:38:PRO:HD3	2.00	0.43
1:B:90:VAL:HG13	1:B:96:VAL:HG11	1.99	0.43
1:B:103:THR:CG2	1:D:117:MSE:HE1	2.49	0.43
1:B:11:ILE:HA	1:B:14:LEU:CD1	2.49	0.43
1:C:23:LEU:HD22	1:C:27:GLU:HB2	2.01	0.43
1:E:74:VAL:HG21	1:E:110:LEU:HD13	2.00	0.43
1:E:139:SER:O	1:G:103:THR:HG22	2.19	0.43
1:E:59:LEU:HD21	1:F:14:LEU:HD22	2.00	0.43
1:E:37:SER:N	1:E:38:PRO:HD2	2.33	0.43
1:G:2:PRO:CG	1:H:65:ASN:HD22	2.32	0.43
1:H:86:PHE:O	1:H:90:VAL:HG22	2.19	0.43
1:A:62:GLU:CD	1:A:62:GLU:H	2.27	0.42
1:B:76:ILE:HG22	1:B:77:ARG:O	2.19	0.42
1:B:4:LEU:HD22	1:B:42:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ILE:HG23	1:E:139:SER:HB3	2.01	0.42
1:B:117:MSE:CE	1:G:117:MSE:CE	2.97	0.42
1:D:45:GLN:O	1:D:49:ALA:HB2	2.20	0.42
1:E:27:GLU:O	1:E:30:GLU:HG2	2.19	0.42
1:G:13:ILE:CD1	1:G:32:VAL:HG21	2.47	0.42
1:A:65:ASN:HD21	3:A:803:GOL:C1	2.32	0.42
1:C:16:VAL:HG11	1:C:31:ARG:HD2	2.01	0.42
1:H:120:PHE:CE2	1:H:124:VAL:HG11	2.54	0.42
1:C:107:ASP:O	2:C:1160:MET:HE3	2.20	0.42
1:G:97:LEU:O	1:H:149:THR:HG22	2.18	0.42
1:C:73:ARG:HD2	1:C:106:THR:HG21	2.02	0.41
1:D:11:ILE:HG22	1:D:15:GLN:HG3	2.02	0.41
1:D:73:ARG:CB	1:D:106:THR:HG21	2.50	0.41
1:E:141:PHE:H	1:F:103:THR:HG1	1.63	0.41
1:D:34:LEU:HD22	1:D:39:CYS:N	2.36	0.41
1:D:87:ALA:HB1	1:D:91:ARG:HH12	1.84	0.41
1:G:103:THR:HG22	1:G:104:GLY:N	2.36	0.41
1:A:74:VAL:HG13	1:A:134:VAL:HG13	2.01	0.41
1:C:120:PHE:CZ	1:C:124:VAL:CG2	3.04	0.41
1:B:76:ILE:HD11	1:B:86:PHE:CG	2.55	0.41
1:G:34:LEU:HD13	1:G:39:CYS:HA	2.02	0.41
1:H:45:GLN:O	1:H:49:ALA:N	2.54	0.41
1:A:43:LEU:HD11	1:A:55:TYR:OH	2.21	0.41
1:A:150:THR:HG23	5:B:1181:HOH:O	2.19	0.41
1:F:24:THR:HG23	1:F:27:GLU:CD	2.46	0.41
1:A:35:SER:HB2	1:A:38:PRO:HD2	2.02	0.41
1:A:72:ILE:HD11	1:A:120:PHE:HE1	1.86	0.41
1:H:9:THR:HG21	1:H:34:LEU:HD21	2.02	0.41
1:A:7:ASP:OD1	1:A:7:ASP:C	2.63	0.41
1:A:32:VAL:HG23	1:A:34:LEU:HB2	2.02	0.41
1:D:37:SER:N	1:D:38:PRO:CD	2.84	0.41
1:H:128:LEU:HD13	1:H:134:VAL:HG21	2.02	0.41
1:B:73:ARG:CG	1:B:106:THR:HG21	2.51	0.41
1:G:18:GLN:HE22	1:G:152:LEU:H	1.69	0.41
1:H:117:MSE:HB2	3:H:809:GOL:O1	2.20	0.41
1:C:18:GLN:OE1	1:D:59:LEU:HD12	2.20	0.40
1:F:13:ILE:HG13	1:F:32:VAL:HG11	2.03	0.40
1:F:58:LEU:CD1	1:F:150:THR:CG2	2.99	0.40
1:B:92:LYS:O	1:B:94:PRO:HD3	2.22	0.40
1:B:117:MSE:HE1	1:G:117:MSE:CE	2.51	0.40
1:E:79:ALA:C	1:E:81:ASP:H	2.29	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	154/162 (95%)	145 (94%)	8 (5%)	1 (1%)	21	51
1	B	154/162 (95%)	147 (96%)	6 (4%)	1 (1%)	21	51
1	C	152/162 (94%)	140 (92%)	12 (8%)	0	100	100
1	D	154/162 (95%)	143 (93%)	8 (5%)	3 (2%)	6	22
1	E	154/162 (95%)	147 (96%)	7 (4%)	0	100	100
1	F	152/162 (94%)	144 (95%)	8 (5%)	0	100	100
1	G	156/162 (96%)	148 (95%)	8 (5%)	0	100	100
1	H	152/162 (94%)	146 (96%)	6 (4%)	0	100	100
All	All	1228/1296 (95%)	1160 (94%)	63 (5%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	81	ASP
1	D	49	ALA
1	A	31	ARG
1	B	65	ASN
1	D	36	PRO

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	138/141 (98%)	131 (95%)	7 (5%)	21	54
1	B	138/141 (98%)	126 (91%)	12 (9%)	9	30
1	C	136/141 (96%)	123 (90%)	13 (10%)	8	26
1	D	138/141 (98%)	131 (95%)	7 (5%)	21	54
1	E	138/141 (98%)	132 (96%)	6 (4%)	26	60
1	F	136/141 (96%)	127 (93%)	9 (7%)	15	43
1	G	140/141 (99%)	131 (94%)	9 (6%)	16	44
1	H	136/141 (96%)	127 (93%)	9 (7%)	15	43
All	All	1100/1128 (98%)	1028 (94%)	72 (6%)	15	43

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	31	ARG
1	A	39	CYS
1	A	42	ARG
1	A	84	GLU
1	A	89	SER
1	A	142	VAL
1	B	11	ILE
1	B	15	GLN
1	B	34	LEU
1	B	37	SER
1	B	43	LEU
1	B	45	GLN
1	B	77	ARG
1	B	78	LYS
1	B	89	SER
1	B	102	LEU
1	B	109	LEU
1	B	115	THR
1	C	5	THR
1	C	6	LEU
1	C	8	LYS
1	C	9	THR
1	C	12	LYS
1	C	20	ASN
1	C	37	SER
1	C	40	LEU

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Mol	Chain	Res	Type
1	C	65	ASN
1	C	78	LYS
1	C	98	SER
1	C	106	THR
1	C	118	ASN
1	D	4	LEU
1	D	6	LEU
1	D	9	THR
1	D	48	ASP
1	D	76	ILE
1	D	95	GLU
1	D	115	THR
1	E	51	ILE
1	E	76	ILE
1	E	92	LYS
1	E	95	GLU
1	E	106	THR
1	E	156	HIS
1	F	24	THR
1	F	63	SER
1	F	74	VAL
1	F	95	GLU
1	F	106	THR
1	F	110	LEU
1	F	115	THR
1	F	144	LYS
1	F	150	THR
1	G	8	LYS
1	G	32	VAL
1	G	34	LEU
1	G	60	SER
1	G	65	ASN
1	G	68	LEU
1	G	73	ARG
1	G	95	GLU
1	G	110	LEU
1	H	6	LEU
1	H	23	LEU
1	H	39	CYS
1	H	73	ARG
1	H	95	GLU
1	H	98	SER

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Mol	Chain	Res	Type
1	H	115	THR
1	H	122	HIS
1	H	128	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	69	GLN
1	A	111	GLN
1	A	135	GLN
1	A	148	HIS
1	B	15	GLN
1	B	69	GLN
1	B	135	GLN
1	B	155	ASN
1	C	20	ASN
1	C	45	GLN
1	C	54	GLN
1	C	111	GLN
1	D	18	GLN
1	D	54	GLN
1	E	45	GLN
1	E	54	GLN
1	E	111	GLN
1	F	25	ASN
1	F	54	GLN
1	F	69	GLN
1	F	111	GLN
1	F	135	GLN
1	F	138	GLN
1	F	155	ASN
1	G	15	GLN
1	G	18	GLN
1	G	25	ASN
1	H	65	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 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	$\# Z > 2$
3	GOL	F	806	-	5,5,5	0.41	0	5,5,5	0.25	0
2	MET	C	1160	-	7,8,8	0.93	1 (14%)	5,9,9	1.47	1 (20%)
2	MET	D	1160	-	7,8,8	0.91	1 (14%)	5,9,9	1.27	1 (20%)
3	GOL	A	901	-	5,5,5	0.38	0	5,5,5	0.31	0
3	GOL	A	904	-	5,5,5	0.45	0	5,5,5	0.33	0
3	GOL	C	807	-	5,5,5	0.41	0	5,5,5	0.13	0
3	GOL	H	809	-	5,5,5	0.39	0	5,5,5	0.61	0
2	MET	H	1160	-	7,8,8	0.95	1 (14%)	5,9,9	1.33	1 (20%)
2	MET	B	1160	-	7,8,8	0.88	1 (14%)	5,9,9	1.37	1 (20%)
2	MET	F	1160	-	7,8,8	0.85	1 (14%)	5,9,9	1.31	1 (20%)
2	MET	G	1160	-	7,8,8	0.97	1 (14%)	5,9,9	1.25	1 (20%)
3	GOL	C	805	-	5,5,5	0.43	0	5,5,5	0.35	0
3	GOL	A	801	-	5,5,5	0.40	0	5,5,5	0.15	0
3	GOL	F	804	-	5,5,5	0.35	0	5,5,5	0.13	0
3	GOL	E	909	-	5,5,5	0.39	0	5,5,5	0.28	0
3	GOL	A	902	-	5,5,5	0.42	0	5,5,5	0.18	0
3	GOL	A	803	-	5,5,5	0.39	0	5,5,5	0.16	0
3	GOL	A	802	-	5,5,5	0.36	0	5,5,5	0.31	0
2	MET	A	1160	-	7,8,8	0.86	1 (14%)	5,9,9	1.39	1 (20%)
2	MET	E	1160	-	7,8,8	0.87	1 (14%)	5,9,9	1.28	1 (20%)

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	GOL	F	806	-	-	2/4/4/4	-
2	MET	C	1160	-	-	0/8/8/8	-
2	MET	D	1160	-	-	0/8/8/8	-
3	GOL	A	901	-	-	0/4/4/4	-
3	GOL	A	904	-	-	2/4/4/4	-
3	GOL	C	807	-	-	2/4/4/4	-
3	GOL	H	809	-	-	0/4/4/4	-
2	MET	H	1160	-	-	0/8/8/8	-
2	MET	B	1160	-	-	0/8/8/8	-
2	MET	F	1160	-	-	0/8/8/8	-
2	MET	G	1160	-	-	2/8/8/8	-
3	GOL	C	805	-	-	4/4/4/4	-
3	GOL	A	801	-	-	4/4/4/4	-
3	GOL	F	804	-	-	4/4/4/4	-
3	GOL	E	909	-	-	0/4/4/4	-
3	GOL	A	902	-	-	4/4/4/4	-
3	GOL	A	803	-	-	3/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
2	MET	A	1160	-	-	0/8/8/8	-
2	MET	E	1160	-	-	0/8/8/8	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1160	MET	OXT-C	-2.50	1.22	1.30
2	C	1160	MET	OXT-C	-2.39	1.23	1.30
2	H	1160	MET	OXT-C	-2.33	1.23	1.30
2	D	1160	MET	OXT-C	-2.27	1.23	1.30
2	B	1160	MET	OXT-C	-2.25	1.23	1.30
2	E	1160	MET	OXT-C	-2.22	1.23	1.30
2	A	1160	MET	OXT-C	-2.18	1.23	1.30
2	F	1160	MET	OXT-C	-2.16	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1160	MET	OXT-C-O	-3.25	116.71	124.08
2	A	1160	MET	OXT-C-O	-3.04	117.18	124.08
2	B	1160	MET	OXT-C-O	-2.99	117.29	124.08
2	H	1160	MET	OXT-C-O	-2.92	117.47	124.08
2	F	1160	MET	OXT-C-O	-2.89	117.52	124.08
2	E	1160	MET	OXT-C-O	-2.84	117.63	124.08
2	D	1160	MET	OXT-C-O	-2.84	117.63	124.08
2	G	1160	MET	OXT-C-O	-2.67	118.02	124.08

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	GOL	O1-C1-C2-C3
3	A	902	GOL	C1-C2-C3-O3
3	A	904	GOL	O1-C1-C2-C3
3	A	802	GOL	C1-C2-C3-O3
3	A	801	GOL	C1-C2-C3-O3
3	A	803	GOL	C1-C2-C3-O3
3	F	806	GOL	O1-C1-C2-C3
3	F	804	GOL	O1-C1-C2-C3
3	F	804	GOL	C1-C2-C3-O3
3	C	805	GOL	O1-C1-C2-O2
3	F	804	GOL	O1-C1-C2-O2
2	G	1160	MET	OXT-C-CA-N
3	A	801	GOL	O1-C1-C2-C3
3	C	805	GOL	O1-C1-C2-C3
3	C	805	GOL	C1-C2-C3-O3
3	C	807	GOL	O1-C1-C2-C3
3	A	902	GOL	O1-C1-C2-O2
3	A	902	GOL	O2-C2-C3-O3
3	A	801	GOL	O1-C1-C2-O2
3	A	801	GOL	O2-C2-C3-O3
3	A	803	GOL	O2-C2-C3-O3
3	C	807	GOL	O1-C1-C2-O2
3	F	806	GOL	O1-C1-C2-O2
3	F	804	GOL	O2-C2-C3-O3
3	A	904	GOL	O1-C1-C2-O2
2	G	1160	MET	O-C-CA-N
3	A	802	GOL	O2-C2-C3-O3
3	A	803	GOL	O1-C1-C2-C3
3	C	805	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1160	MET	1	0
3	H	809	GOL	3	0
2	F	1160	MET	1	0
2	G	1160	MET	1	0
3	A	803	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	155/162 (95%)	-0.08	0 100 100	20, 66, 90, 100	0
1	B	155/162 (95%)	-0.20	0 100 100	20, 68, 89, 101	0
1	C	153/162 (94%)	-0.23	0 100 100	41, 72, 90, 100	0
1	D	155/162 (95%)	0.10	2 (1%) 75 66	51, 73, 98, 112	0
1	E	155/162 (95%)	-0.15	1 (0%) 85 80	49, 73, 95, 112	0
1	F	153/162 (94%)	-0.17	0 100 100	53, 71, 89, 95	0
1	G	156/162 (96%)	-0.11	0 100 100	52, 76, 97, 141	0
1	H	153/162 (94%)	-0.13	0 100 100	53, 74, 91, 98	0
All	All	1235/1296 (95%)	-0.12	3 (0%) 91 88	20, 72, 94, 141	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	LEU	2.9
1	D	146	ILE	2.3
1	E	9	THR	2.1

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
3	GOL	C	807	6/6	0.43	0.13	109,110,112,116	0
3	GOL	A	803	6/6	0.62	0.11	63,65,65,68	0
3	GOL	A	902	6/6	0.62	0.11	54,77,83,91	0
3	GOL	C	805	6/6	0.63	0.11	71,82,84,85	0
3	GOL	E	909	6/6	0.64	0.13	71,84,91,96	0
3	GOL	A	802	6/6	0.70	0.11	72,80,82,84	0
3	GOL	F	804	6/6	0.70	0.13	61,64,65,65	0
3	GOL	A	801	6/6	0.74	0.11	67,78,80,87	0
3	GOL	A	904	6/6	0.75	0.12	82,85,87,90	0
4	CA	C	161	1/1	0.76	0.08	94,94,94,94	0
3	GOL	H	809	6/6	0.78	0.16	38,56,63,69	0
3	GOL	F	806	6/6	0.81	0.12	74,89,95,101	0
4	CA	F	932	1/1	0.84	0.12	73,73,73,73	0
4	CA	B	961	1/1	0.86	0.07	81,81,81,81	0
4	CA	D	1020	1/1	0.87	0.11	83,83,83,83	0
4	CA	B	978	1/1	0.87	0.07	92,92,92,92	0
2	MET	F	1160	9/9	0.88	0.15	38,47,51,52	0
2	MET	G	1160	9/9	0.88	0.13	48,50,58,59	0
4	CA	B	999	1/1	0.89	0.08	61,61,61,61	0
3	GOL	A	901	6/6	0.89	0.09	38,48,51,53	0
2	MET	E	1160	9/9	0.90	0.15	45,52,55,57	0
2	MET	H	1160	9/9	0.90	0.14	42,45,49,52	0
4	CA	E	227	1/1	0.91	0.09	63,63,63,63	0
2	MET	D	1160	9/9	0.91	0.11	44,47,49,51	0
2	MET	C	1160	9/9	0.92	0.16	47,49,51,51	0
4	CA	F	1050	1/1	0.92	0.06	75,75,75,75	0
2	MET	A	1160	9/9	0.93	0.12	42,47,49,51	0
2	MET	B	1160	9/9	0.95	0.12	42,48,51,51	0
4	CA	E	216	1/1	0.96	0.08	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.