



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:11 AM GMT

PDB ID : 2G0B
Title : The structure of FeeM, an N-acyl amino acid synthase from uncultured soil microbes
Authors : Van Wagoner, R.M.; Clardy, J.
Deposited on : 2006-02-11
Resolution : 3.00 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

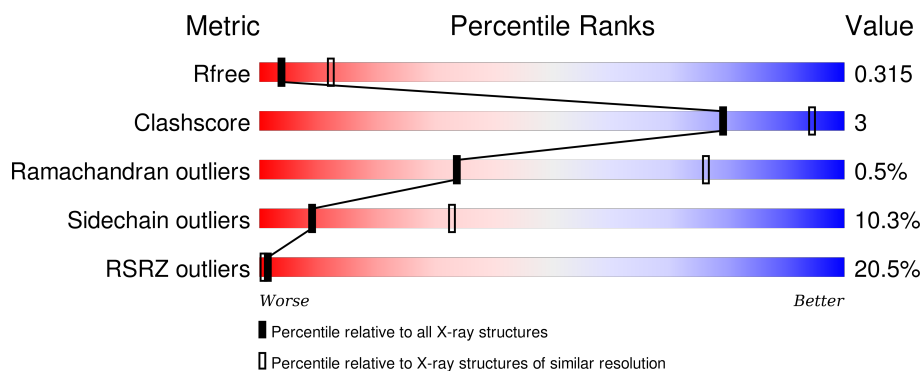
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	198	<div> <div>11%</div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div>
1	B	198	<div> <div>24%</div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div>
1	C	198	<div> <div>23%</div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div>
1	D	198	<div> <div>29%</div> <div>79%</div> <div>10%</div> <div>• 9%</div> </div>
1	E	198	<div> <div>12%</div> <div>75%</div> <div>16%</div> <div>• 9%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	198	
1	G	198	
1	H	198	

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
2	NLT	B	401	-	-	-	X
2	NLT	C	402	-	-	-	X
2	NLT	D	403	-	-	-	X
2	NLT	E	404	-	-	-	X
2	NLT	F	405	-	-	-	X
2	NLT	G	406	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11507 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 FeeM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1461	942	241	272	6			
1	B	189	Total	C	N	O	S	0	0	0
			1468	948	243	272	5			
1	C	184	Total	C	N	O	S	0	0	0
			1427	920	237	266	4			
1	D	181	Total	C	N	O	S	0	0	0
			1413	911	234	263	5			
1	E	181	Total	C	N	O	S	0	0	0
			1413	911	234	263	5			
1	F	184	Total	C	N	O	S	0	0	0
			1427	920	237	266	4			
1	G	174	Total	C	N	O	S	0	0	0
			1345	866	222	253	4			
1	H	170	Total	C	N	O	S	0	0	0
			1336	864	222	245	5			

There are 16 discrepancies between the modelled and reference sequences:

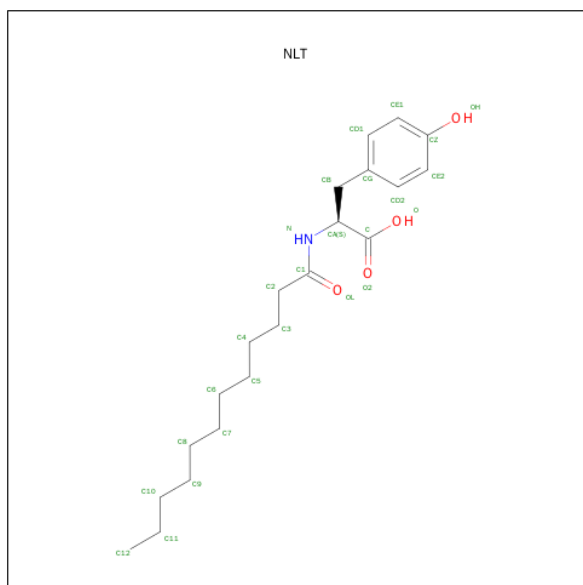
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
A	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
B	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
B	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
C	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
C	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
D	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
D	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
E	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
E	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
F	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
F	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
G	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7
H	-1	GLY	-	CLONING ARTIFACT	UNP Q8KNZ7
H	0	SER	-	CLONING ARTIFACT	UNP Q8KNZ7

- Molecule 2 is N-DODECANOYL-L-TYROSINE (three-letter code: NLT) (formula: $C_{21}H_{33}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	21	1	4		
2	B	1	Total	C	N	O	0	0
			26	21	1	4		
2	C	1	Total	C	N	O	0	0
			26	21	1	4		
2	D	1	Total	C	N	O	0	0
			26	21	1	4		
2	E	1	Total	C	N	O	0	0
			26	21	1	4		
2	F	1	Total	C	N	O	0	0
			26	21	1	4		
2	G	1	Total	C	N	O	0	0
			26	21	1	4		
2	H	1	Total	C	N	O	0	0
			26	21	1	4		

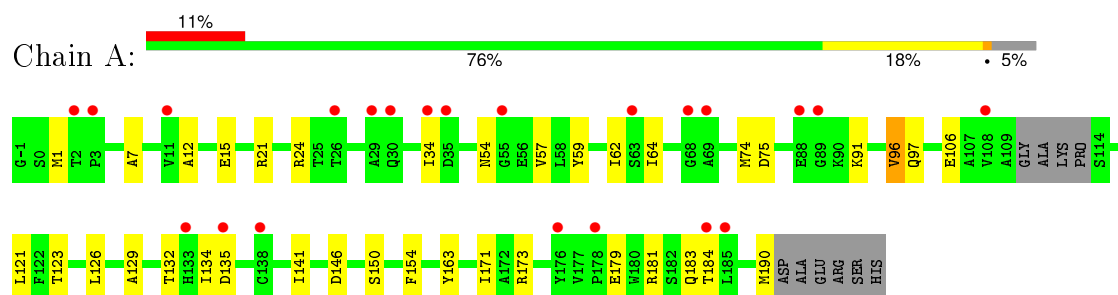
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

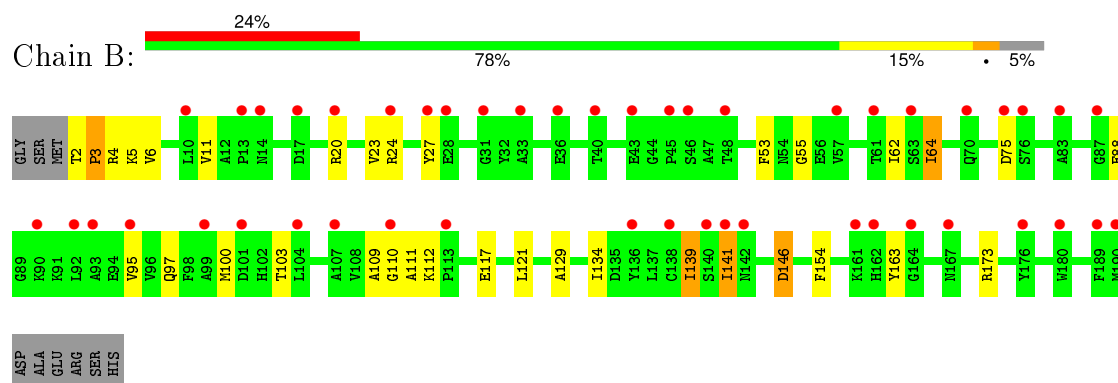
3 Residue-property plots [i](#)

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.

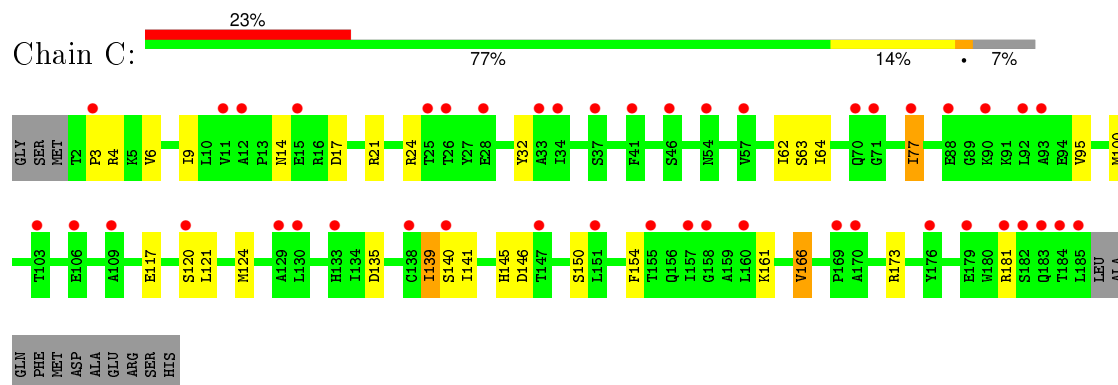
• Molecule 1: FeeM



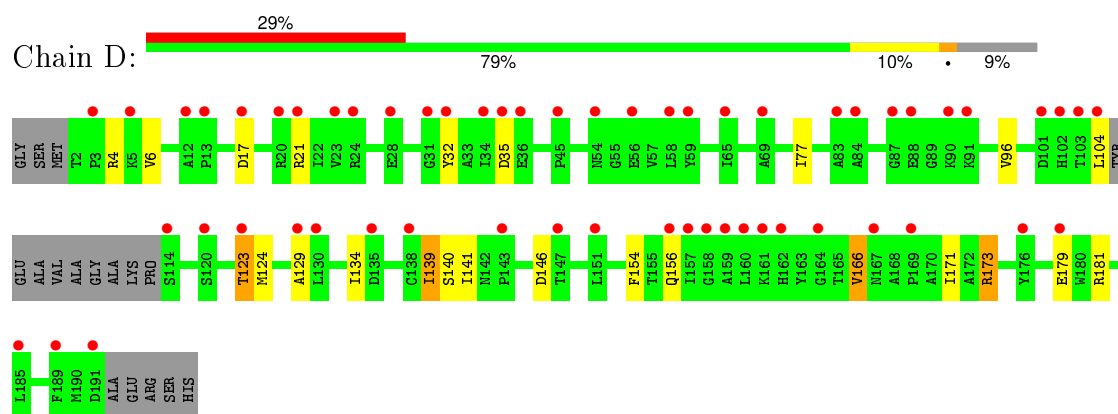
• Molecule 1: FeeM



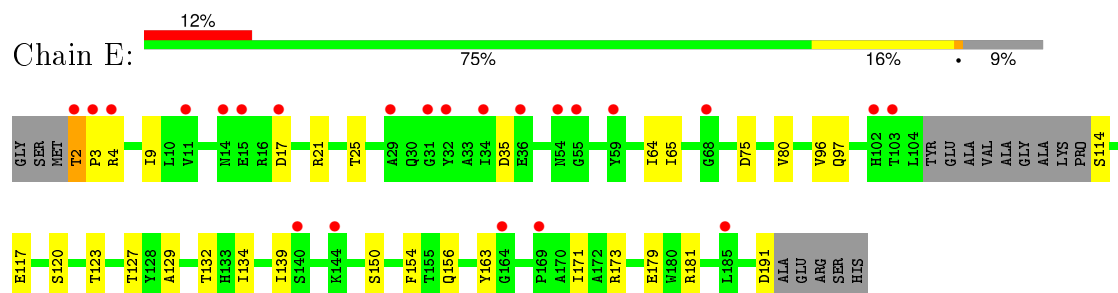
• Molecule 1: FeeM



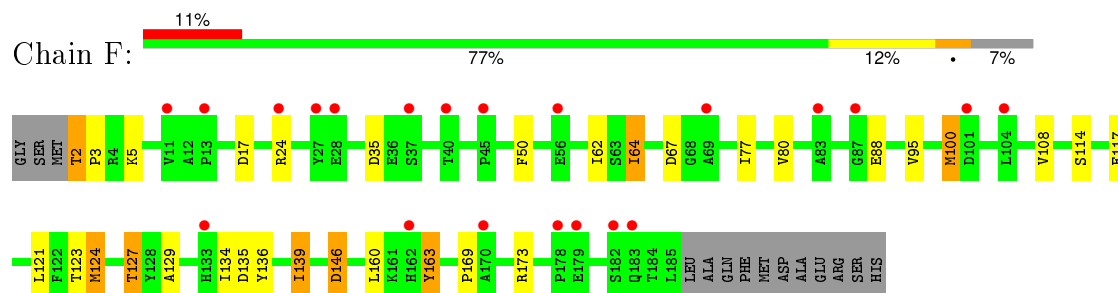
• Molecule 1: FeeM



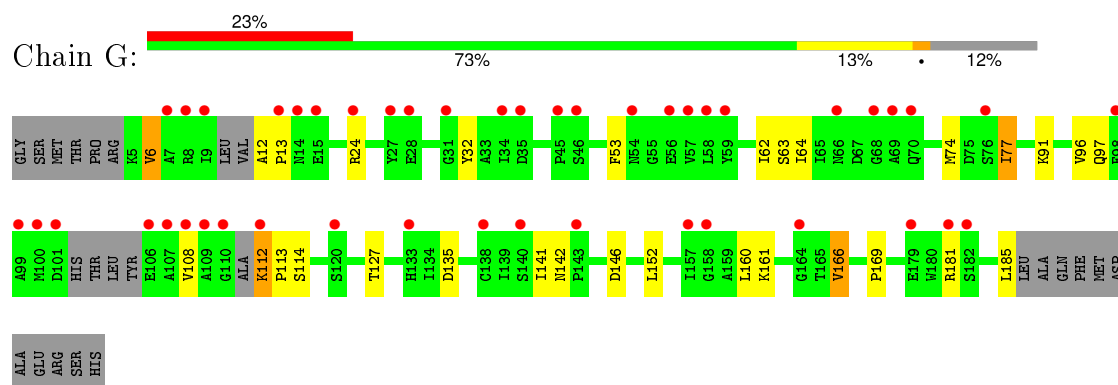
• Molecule 1: FeeM



• Molecule 1: FeeM

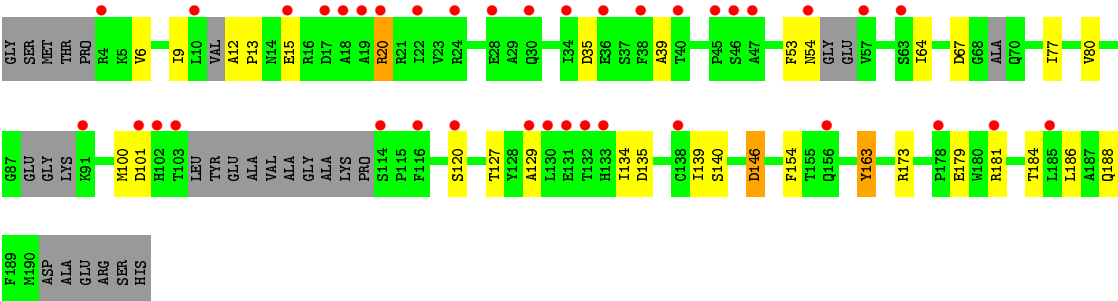


• Molecule 1: FeeM



• Molecule 1: FeeM





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	182.83Å 182.83Å 287.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.00 29.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.75-3.00) 100.0 (29.75-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.255 , 0.292 0.288 , 0.315	Depositor DCC
R_{free} test set	2458 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48827 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	11507	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NLT

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	0.55	0/1495	0.66	2/2033 (0.1%)
1	B	0.53	0/1504	0.65	2/2048 (0.1%)
1	C	0.45	0/1462	0.64	3/1992 (0.2%)
1	D	0.46	0/1446	0.64	3/1967 (0.2%)
1	E	0.47	0/1446	0.64	4/1967 (0.2%)
1	F	0.52	0/1462	0.65	3/1992 (0.2%)
1	G	0.43	0/1374	0.62	2/1865 (0.1%)
1	H	0.43	0/1364	0.62	5/1849 (0.3%)
All	All	0.48	0/11553	0.64	24/15713 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	35	ASP	CB-CG-OD2	5.89	123.60	118.30
1	G	146	ASP	CB-CG-OD2	5.64	123.37	118.30
1	E	191	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	35	ASP	CB-CG-OD2	5.55	123.29	118.30
1	E	75	ASP	CB-CG-OD2	5.40	123.16	118.30
1	H	146	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	35	ASP	CB-CG-OD2	5.35	123.11	118.30
1	F	135	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	67	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	75	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	17	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	17	ASP	CB-CG-OD2	5.26	123.03	118.30
1	G	135	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	146	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	135	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	17	ASP	CB-CG-OD2	5.15	122.93	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	146	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	17	ASP	CB-CG-OD2	5.08	122.87	118.30
1	H	135	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	146	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	135	ASP	CB-CG-OD2	5.02	122.82	118.30
1	H	101	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	75	ASP	CB-CG-OD2	5.00	122.80	118.30

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	1461	0	1443	12	0
1	B	1468	0	1452	17	0
1	C	1427	0	1410	9	0
1	D	1413	0	1393	6	0
1	E	1413	0	1393	9	0
1	F	1427	0	1410	15	1
1	G	1345	0	1321	9	0
1	H	1336	0	1315	9	0
2	A	26	0	31	1	0
2	B	26	0	31	1	0
2	C	26	0	31	0	0
2	D	26	0	31	1	0
2	E	26	0	31	0	0
2	F	26	0	31	1	0
2	G	26	0	31	1	0
2	H	26	0	31	0	0
3	A	9	0	0	0	0
All	All	11507	0	11385	79	1

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 3.

All (79) 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:B:2:THR:HB	1:B:3:PRO:HD2	1.39	1.03
1:B:23:VAL:HG21	1:B:97:GLN:HG3	1.69	0.74
1:G:6:VAL:HG23	1:G:53:PHE:HB2	1.73	0.71
1:B:2:THR:CB	1:B:3:PRO:HD2	2.19	0.71
1:G:96:VAL:HG22	1:G:97:GLN:HG2	1.73	0.71
1:A:146:ASP:OD2	1:A:173:ARG:NH1	2.27	0.68
1:H:77:ILE:HD11	1:H:163:TYR:HA	1.78	0.66
1:B:27:TYR:OH	2:B:401:NLT:O2	2.18	0.62
1:A:91:LYS:HE2	1:A:132:THR:HG22	1.82	0.61
1:D:154:PHE:HB3	1:D:173:ARG:HB3	1.83	0.61
1:F:146:ASP:OD2	1:F:173:ARG:NH1	2.37	0.58
1:E:156:GLN:HB2	1:E:173:ARG:HH21	1.69	0.58
1:H:184:THR:HG22	1:H:186:LEU:H	1.71	0.56
1:B:109:ALA:O	1:B:111:ALA:N	2.37	0.56
1:A:123:THR:HG21	1:B:117:GLU:OE2	2.05	0.56
1:A:7:ALA:HB3	1:B:5:LYS:HB2	1.88	0.55
1:F:62:ILE:HG22	1:F:121:LEU:HD22	1.90	0.53
1:E:96:VAL:HG22	1:E:97:GLN:HG2	1.90	0.53
1:C:32:TYR:HB3	1:C:166:VAL:HG22	1.90	0.53
1:C:117:GLU:OE2	1:D:123:THR:HG21	2.07	0.53
1:G:77:ILE:HG23	1:G:161:LYS:HD2	1.90	0.52
1:H:146:ASP:OD1	1:H:173:ARG:NH1	2.41	0.52
1:A:129:ALA:HA	1:A:134:ILE:HD12	1.92	0.52
1:C:77:ILE:HG23	1:C:161:LYS:HD2	1.90	0.51
1:F:77:ILE:CD1	1:F:163:TYR:HA	2.40	0.51
1:B:154:PHE:HB3	1:B:173:ARG:HB3	1.93	0.50
1:G:32:TYR:HB3	1:G:166:VAL:HG22	1.92	0.50
1:E:9:ILE:HD11	1:F:2:THR:HG23	1.93	0.50
1:F:64:ILE:HG22	1:F:95:VAL:HG13	1.93	0.49
1:B:62:ILE:HG22	1:B:121:LEU:HD22	1.95	0.49
1:A:12:ALA:HB3	1:A:15:GLU:HG3	1.96	0.48
1:E:154:PHE:HB3	1:E:173:ARG:HB3	1.94	0.48
1:D:139:ILE:HD11	2:D:403:NLT:H62	1.96	0.48
1:B:2:THR:HB	1:B:3:PRO:CD	2.28	0.48
1:G:62:ILE:HD11	2:G:406:NLT:H52	1.95	0.47
1:E:123:THR:HG21	1:F:117:GLU:OE2	2.15	0.47
1:F:100:MET:HE3	1:F:100:MET:HB3	1.73	0.47
1:F:50:PHE:CD2	1:F:124:MET:HG2	2.49	0.47
1:H:154:PHE:HB3	1:H:173:ARG:HB3	1.95	0.47
1:A:96:VAL:HG13	1:A:97:GLN:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HG23	1:B:141:ILE:HG23	1.97	0.47
1:G:112:LYS:HE2	1:G:113:PRO:HD2	1.96	0.46
1:F:139:ILE:HD11	2:F:405:NLT:H71	1.96	0.46
1:C:6:VAL:HG13	1:D:6:VAL:HG22	1.97	0.46
1:B:129:ALA:HA	1:B:134:ILE:HD12	1.97	0.46
1:B:95:VAL:HB	1:B:139:ILE:HD11	1.97	0.45
1:G:160:LEU:HD11	1:G:169:PRO:HB3	1.97	0.45
1:C:95:VAL:HB	1:C:139:ILE:HD11	1.97	0.45
1:H:6:VAL:HB	1:H:53:PHE:HB2	1.98	0.45
1:B:146:ASP:OD2	1:B:173:ARG:NH1	2.49	0.45
1:D:129:ALA:HA	1:D:134:ILE:HD12	1.98	0.45
1:B:6:VAL:HB	1:B:53:PHE:HB2	1.99	0.44
1:A:62:ILE:HG22	1:A:121:LEU:HD22	2.00	0.44
1:D:32:TYR:HB3	1:D:166:VAL:HG22	1.99	0.44
1:B:64:ILE:HG22	1:B:95:VAL:HG13	2.01	0.43
1:H:129:ALA:HA	1:H:134:ILE:HD12	2.01	0.42
1:A:24:ARG:HG3	1:A:34:ILE:HD13	2.01	0.42
1:C:154:PHE:HB3	1:C:173:ARG:HB3	2.02	0.42
1:G:152:LEU:HA	1:G:152:LEU:HD23	1.89	0.42
1:C:62:ILE:HG22	1:C:121:LEU:HD22	2.01	0.42
1:E:2:THR:HA	1:E:3:PRO:HD3	1.91	0.42
1:A:126:LEU:HD13	2:A:400:NLT:H121	2.01	0.42
1:H:12:ALA:HA	1:H:13:PRO:HD3	1.91	0.42
1:F:160:LEU:HD11	1:F:169:PRO:HB3	2.02	0.42
1:F:123:THR:O	1:F:127:THR:OG1	2.36	0.42
1:A:154:PHE:HB3	1:A:173:ARG:HB3	2.02	0.41
1:E:129:ALA:HA	1:E:134:ILE:HD12	2.03	0.41
1:A:54:ASN:HB2	1:A:59:TYR:CD2	2.55	0.41
1:C:139:ILE:HG23	1:C:141:ILE:HG23	2.01	0.41
1:F:129:ALA:HA	1:F:134:ILE:HD12	2.02	0.41
1:F:77:ILE:HD12	1:F:163:TYR:HA	2.03	0.41
1:H:12:ALA:HB3	1:H:15:GLU:HB2	2.02	0.41
1:H:20:ARG:HH21	1:H:39:ALA:HB1	1.85	0.41
1:B:2:THR:CB	1:B:3:PRO:CD	2.93	0.41
1:E:65:ILE:HD12	1:E:96:VAL:HG11	2.02	0.41
1:F:77:ILE:HG21	1:F:77:ILE:HD13	1.82	0.40
1:C:139:ILE:HD13	1:C:139:ILE:HA	1.78	0.40
1:E:117:GLU:HG3	1:F:123:THR:HG21	2.04	0.40
1:G:12:ALA:HA	1:G:13:PRO:HD3	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:GLU:OE2	1:F:136:TYR:OH[6_565]	2.05	0.15

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	184/198 (93%)	176 (96%)	7 (4%)	1 (0%)	34	76
1	B	187/198 (94%)	182 (97%)	2 (1%)	3 (2%)	12	48
1	C	182/198 (92%)	177 (97%)	4 (2%)	1 (0%)	34	76
1	D	177/198 (89%)	169 (96%)	8 (4%)	0	100	100
1	E	177/198 (89%)	174 (98%)	3 (2%)	0	100	100
1	F	182/198 (92%)	174 (96%)	6 (3%)	2 (1%)	17	58
1	G	166/198 (84%)	157 (95%)	9 (5%)	0	100	100
1	H	158/198 (80%)	153 (97%)	5 (3%)	0	100	100
All	All	1413/1584 (89%)	1362 (96%)	44 (3%)	7 (0%)	34	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	GLY
1	B	3	PRO
1	C	3	PRO
1	A	106	GLU
1	F	67	ASP
1	B	55	GLY
1	F	3	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	150/157 (96%)	135 (90%)	15 (10%)	9	34
1	B	150/157 (96%)	138 (92%)	12 (8%)	15	47
1	C	146/157 (93%)	129 (88%)	17 (12%)	7	27
1	D	146/157 (93%)	130 (89%)	16 (11%)	8	30
1	E	146/157 (93%)	130 (89%)	16 (11%)	8	30
1	F	146/157 (93%)	133 (91%)	13 (9%)	12	42
1	G	137/157 (87%)	121 (88%)	16 (12%)	7	27
1	H	138/157 (88%)	124 (90%)	14 (10%)	9	34
All	All	1159/1256 (92%)	1040 (90%)	119 (10%)	9	33

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	ARG
1	A	57	VAL
1	A	64	ILE
1	A	74	MET
1	A	96	VAL
1	A	141	ILE
1	A	150	SER
1	A	163	TYR
1	A	171	ILE
1	A	179	GLU
1	A	181	ARG
1	A	183	GLN
1	A	184	THR
1	A	190	MET
1	B	4	ARG
1	B	11	VAL
1	B	20	ARG
1	B	24	ARG
1	B	64	ILE
1	B	88	GLU
1	B	100	MET
1	B	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	112	LYS
1	B	139	ILE
1	B	141	ILE
1	B	163	TYR
1	C	4	ARG
1	C	9	ILE
1	C	14	ASN
1	C	21	ARG
1	C	24	ARG
1	C	63	SER
1	C	64	ILE
1	C	77	ILE
1	C	100	MET
1	C	120	SER
1	C	124	MET
1	C	139	ILE
1	C	140	SER
1	C	145	HIS
1	C	150	SER
1	C	166	VAL
1	C	181	ARG
1	D	4	ARG
1	D	21	ARG
1	D	77	ILE
1	D	96	VAL
1	D	104	LEU
1	D	123	THR
1	D	124	MET
1	D	139	ILE
1	D	140	SER
1	D	141	ILE
1	D	156	GLN
1	D	166	VAL
1	D	171	ILE
1	D	173	ARG
1	D	179	GLU
1	D	181	ARG
1	E	2	THR
1	E	4	ARG
1	E	21	ARG
1	E	25	THR
1	E	64	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	80	VAL
1	E	114	SER
1	E	120	SER
1	E	127	THR
1	E	132	THR
1	E	139	ILE
1	E	150	SER
1	E	163	TYR
1	E	171	ILE
1	E	179	GLU
1	E	181	ARG
1	F	2	THR
1	F	5	LYS
1	F	24	ARG
1	F	35	ASP
1	F	64	ILE
1	F	80	VAL
1	F	100	MET
1	F	108	VAL
1	F	114	SER
1	F	124	MET
1	F	127	THR
1	F	139	ILE
1	F	163	TYR
1	G	6	VAL
1	G	24	ARG
1	G	63	SER
1	G	64	ILE
1	G	74	MET
1	G	77	ILE
1	G	91	LYS
1	G	108	VAL
1	G	112	LYS
1	G	114	SER
1	G	127	THR
1	G	141	ILE
1	G	142	ASN
1	G	166	VAL
1	G	181	ARG
1	G	185	LEU
1	H	9	ILE
1	H	20	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	54	ASN
1	H	64	ILE
1	H	80	VAL
1	H	100	MET
1	H	120	SER
1	H	127	THR
1	H	139	ILE
1	H	140	SER
1	H	163	TYR
1	H	179	GLU
1	H	181	ARG
1	H	188	GLN

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

Mol	Chain	Res	Type
1	C	54	ASN
1	G	142	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NLT	A	400	-	23,26,26	0.47	0	26,31,31	0.72	1 (3%)
2	NLT	B	401	-	23,26,26	0.58	0	26,31,31	0.86	1 (3%)
2	NLT	C	402	-	23,26,26	0.55	0	26,31,31	0.78	1 (3%)
2	NLT	D	403	-	23,26,26	0.57	0	26,31,31	0.91	1 (3%)
2	NLT	E	404	-	23,26,26	0.56	0	26,31,31	0.79	1 (3%)
2	NLT	F	405	-	23,26,26	0.61	0	26,31,31	0.69	1 (3%)
2	NLT	G	406	-	23,26,26	0.58	0	26,31,31	0.97	1 (3%)
2	NLT	H	407	-	23,26,26	0.50	0	26,31,31	0.74	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
2	NLT	A	400	-	-	0/19/23/23	0/1/1/1
2	NLT	B	401	-	-	0/19/23/23	0/1/1/1
2	NLT	C	402	-	-	0/19/23/23	0/1/1/1
2	NLT	D	403	-	-	0/19/23/23	0/1/1/1
2	NLT	E	404	-	-	0/19/23/23	0/1/1/1
2	NLT	F	405	-	-	0/19/23/23	0/1/1/1
2	NLT	G	406	-	-	0/19/23/23	0/1/1/1
2	NLT	H	407	-	-	0/19/23/23	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	406	NLT	CB-CA-C	-3.06	104.97	111.55
2	D	403	NLT	CB-CA-C	-2.81	105.53	111.55
2	B	401	NLT	CB-CA-C	-2.69	105.77	111.55
2	E	404	NLT	CB-CA-C	-2.59	105.99	111.55
2	C	402	NLT	CB-CA-C	-2.36	106.48	111.55
2	A	400	NLT	CB-CA-C	-2.23	106.75	111.55
2	F	405	NLT	CB-CA-C	-2.18	106.87	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NLT	1	0
2	B	401	NLT	1	0
2	D	403	NLT	1	0
2	F	405	NLT	1	0
2	G	406	NLT	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	188/198 (94%)	1.01	22 (11%) 6 2	40, 40, 42, 43	0
1	B	189/198 (95%)	1.33	47 (24%) 1 1	40, 40, 41, 44	0
1	C	184/198 (92%)	1.36	45 (24%) 1 1	40, 40, 41, 41	0
1	D	181/198 (91%)	1.61	57 (31%) 1 0	40, 40, 41, 41	0
1	E	181/198 (91%)	0.86	23 (12%) 5 2	40, 40, 41, 42	0
1	F	184/198 (92%)	0.91	21 (11%) 7 2	40, 40, 41, 42	0
1	G	174/198 (87%)	1.51	45 (25%) 1 1	40, 40, 41, 41	0
1	H	170/198 (85%)	1.32	38 (22%) 1 1	40, 40, 41, 41	0
All	All	1451/1584 (91%)	1.24	298 (20%) 1 1	40, 40, 41, 44	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	47	ALA	9.1
1	D	102	HIS	7.4
1	G	106	GLU	6.3
1	G	54	ASN	6.2
1	E	55	GLY	6.0
1	D	87	GLY	5.9
1	G	182	SER	5.9
1	G	164	GLY	5.9
1	A	26	THR	5.8
1	D	84	ALA	5.6
1	G	112	LYS	5.6
1	G	109	ALA	5.3
1	G	108	VAL	5.3
1	H	17	ASP	5.2
1	H	38	PHE	5.1
1	E	68	GLY	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	56	GLU	5.0
1	C	182	SER	4.9
1	G	28	GLU	4.8
1	G	58	LEU	4.7
1	D	24	ARG	4.7
1	A	29	ALA	4.6
1	D	88	GLU	4.6
1	B	24	ARG	4.5
1	G	110	GLY	4.5
1	H	102	HIS	4.5
1	G	45	PRO	4.4
1	B	13	PRO	4.4
1	H	22	ILE	4.3
1	H	15	GLU	4.3
1	A	69	ALA	4.3
1	H	133	HIS	4.3
1	H	178	PRO	4.3
1	D	56	GLU	4.2
1	G	9	ILE	4.2
1	D	35	ASP	4.2
1	D	147	THR	4.2
1	F	28	GLU	4.1
1	B	28	GLU	4.1
1	C	179	GLU	4.1
1	A	2	THR	4.1
1	E	103	THR	4.1
1	G	27	TYR	4.1
1	E	3	PRO	4.1
1	D	185	LEU	4.1
1	D	83	ALA	4.1
1	B	167	ASN	4.0
1	G	8	ARG	4.0
1	D	162	HIS	4.0
1	C	151	LEU	4.0
1	C	176	TYR	4.0
1	D	58	LEU	4.0
1	A	55	GLY	3.9
1	C	185	LEU	3.9
1	F	45	PRO	3.9
1	D	120	SER	3.9
1	G	57	VAL	3.9
1	D	156	GLN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	100	MET	3.8
1	E	185	LEU	3.8
1	F	69	ALA	3.8
1	C	33	ALA	3.7
1	C	160	LEU	3.7
1	F	87	GLY	3.7
1	B	93	ALA	3.7
1	B	162	HIS	3.7
1	B	87	GLY	3.6
1	D	143	PRO	3.6
1	C	138	CYS	3.6
1	D	45	PRO	3.6
1	C	46	SER	3.6
1	F	11	VAL	3.6
1	A	3	PRO	3.6
1	B	136	TYR	3.5
1	D	103	THR	3.5
1	D	138	CYS	3.5
1	F	56	GLU	3.5
1	H	185	LEU	3.5
1	D	129	ALA	3.5
1	G	138	CYS	3.5
1	C	133	HIS	3.5
1	G	34	ILE	3.5
1	B	113	PRO	3.4
1	H	30	GLN	3.4
1	G	76	SER	3.4
1	E	34	ILE	3.3
1	B	107	ALA	3.3
1	C	41	PHE	3.3
1	E	29	ALA	3.3
1	C	28	GLU	3.3
1	D	20	ARG	3.3
1	G	66	ASN	3.3
1	H	101	ASP	3.3
1	C	183	GLN	3.3
1	G	69	ALA	3.2
1	E	11	VAL	3.2
1	H	18	ALA	3.2
1	H	19	ALA	3.2
1	H	57	VAL	3.2
1	D	90	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	101	ASP	3.2
1	F	101	ASP	3.2
1	B	90	LYS	3.2
1	H	46	SER	3.2
1	B	20	ARG	3.2
1	D	13	PRO	3.1
1	B	61	THR	3.1
1	E	54	ASN	3.1
1	G	133	HIS	3.1
1	D	3	PRO	3.1
1	C	109	ALA	3.1
1	D	158	GLY	3.1
1	B	138	CYS	3.1
1	C	34	ILE	3.1
1	F	183	GLN	3.1
1	H	20	ARG	3.1
1	C	140	SER	3.0
1	G	157	ILE	3.0
1	H	40	THR	3.0
1	E	14	ASN	3.0
1	G	70	GLN	3.0
1	E	32	TYR	3.0
1	C	15	GLU	2.9
1	F	40	THR	2.9
1	D	28	GLU	2.9
1	D	23	VAL	2.9
1	E	169	PRO	2.9
1	H	45	PRO	2.9
1	C	103	THR	2.9
1	H	116	PHE	2.9
1	C	120	SER	2.9
1	D	17	ASP	2.9
1	B	63	SER	2.9
1	E	164	GLY	2.9
1	B	36	GLU	2.8
1	D	161	LYS	2.8
1	C	57	VAL	2.8
1	H	36	GLU	2.8
1	H	131	GLU	2.8
1	D	34	ILE	2.8
1	A	63	SER	2.8
1	C	54	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	101	ASP	2.8
1	C	88	GLU	2.8
1	D	32	TYR	2.8
1	B	70	GLN	2.8
1	H	24	ARG	2.8
1	C	169	PRO	2.8
1	F	27	TYR	2.8
1	D	191	ASP	2.7
1	G	107	ALA	2.7
1	D	54	ASN	2.7
1	H	10	LEU	2.7
1	B	40	THR	2.7
1	G	31	GLY	2.7
1	G	98	PHE	2.7
1	B	83	ALA	2.7
1	H	91	LYS	2.7
1	B	17	ASP	2.7
1	C	184	THR	2.7
1	B	76	SER	2.6
1	C	11	VAL	2.6
1	B	43	GLU	2.6
1	B	140	SER	2.6
1	B	189	PHE	2.6
1	D	59	TYR	2.6
1	E	17	ASP	2.6
1	H	28	GLU	2.6
1	D	12	ALA	2.6
1	B	14	ASN	2.6
1	D	31	GLY	2.6
1	E	102	HIS	2.6
1	F	182	SER	2.6
1	A	185	LEU	2.6
1	H	103	THR	2.6
1	H	156	GLN	2.6
1	G	14	ASN	2.6
1	A	135	ASP	2.6
1	G	181	ARG	2.6
1	D	160	LEU	2.5
1	D	114	SER	2.5
1	A	34	ILE	2.5
1	G	13	PRO	2.5
1	C	70	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	169	PRO	2.5
1	D	135	ASP	2.5
1	F	24	ARG	2.5
1	C	26	THR	2.5
1	E	36	GLU	2.5
1	C	130	LEU	2.5
1	C	181	ARG	2.5
1	F	133	HIS	2.5
1	H	138	CYS	2.5
1	G	140	SER	2.5
1	B	190	MET	2.5
1	B	180	TRP	2.4
1	B	95	VAL	2.4
1	A	108	VAL	2.4
1	G	15	GLU	2.4
1	C	155	THR	2.4
1	H	54	ASN	2.4
1	B	31	GLY	2.4
1	B	57	VAL	2.4
1	C	106	GLU	2.4
1	G	179	GLU	2.4
1	B	46	SER	2.4
1	H	34	ILE	2.4
1	B	33	ALA	2.4
1	C	37	SER	2.4
1	E	144	LYS	2.4
1	A	30	GLN	2.4
1	B	104	LEU	2.4
1	G	59	TYR	2.3
1	A	68	GLY	2.3
1	A	178	PRO	2.3
1	C	147	THR	2.3
1	D	159	ALA	2.3
1	G	7	ALA	2.3
1	B	142	ASN	2.3
1	D	167	ASN	2.3
1	D	179	GLU	2.3
1	G	68	GLY	2.3
1	B	141	ILE	2.3
1	E	31	GLY	2.3
1	F	13	PRO	2.3
1	F	83	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	164	GLY	2.3
1	G	99	ALA	2.3
1	C	92	LEU	2.3
1	D	151	LEU	2.3
1	C	90	LYS	2.3
1	B	101	ASP	2.3
1	E	4	ARG	2.3
1	C	77	ILE	2.3
1	D	176	TYR	2.3
1	F	104	LEU	2.3
1	A	35	ASP	2.2
1	B	45	PRO	2.2
1	B	99	ALA	2.2
1	G	46	SER	2.2
1	H	181	ARG	2.2
1	F	178	PRO	2.2
1	C	93	ALA	2.2
1	D	164	GLY	2.2
1	B	10	LEU	2.2
1	F	170	ALA	2.2
1	H	129	ALA	2.2
1	D	91	LYS	2.2
1	C	129	ALA	2.2
1	C	158	GLY	2.2
1	F	37	SER	2.2
1	B	92	LEU	2.2
1	A	133	HIS	2.2
1	E	15	GLU	2.1
1	D	69	ALA	2.1
1	H	63	SER	2.1
1	E	2	THR	2.1
1	G	35	ASP	2.1
1	G	158	GLY	2.1
1	D	123	THR	2.1
1	D	36	GLU	2.1
1	G	143	PRO	2.1
1	H	4	ARG	2.1
1	B	110	GLY	2.1
1	C	170	ALA	2.1
1	D	157	ILE	2.1
1	D	5	LYS	2.1
1	C	71	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	CYS	2.1
1	B	176	TYR	2.1
1	C	3	PRO	2.1
1	H	120	SER	2.1
1	B	27	TYR	2.1
1	F	162	HIS	2.1
1	D	104	LEU	2.1
1	H	130	LEU	2.1
1	D	21	ARG	2.1
1	E	59	TYR	2.1
1	A	89	GLY	2.1
1	B	161	LYS	2.1
1	A	184	THR	2.1
1	G	120	SER	2.0
1	A	88	GLU	2.0
1	F	179	GLU	2.0
1	H	114	SER	2.0
1	A	176	TYR	2.0
1	D	130	LEU	2.0
1	D	189	PHE	2.0
1	C	25	THR	2.0
1	H	132	THR	2.0
1	G	24	ARG	2.0
1	B	75	ASP	2.0
1	B	48	THR	2.0
1	A	11	VAL	2.0
1	E	140	SER	2.0
1	C	12	ALA	2.0
1	C	157	ILE	2.0
1	D	65	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

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
2	NLT	B	401	26/26	0.60	0.53	2.23	37,40,41,42	0
2	NLT	D	403	26/26	0.60	0.49	1.89	39,41,41,41	0
2	NLT	G	406	26/26	0.69	0.51	1.59	39,40,40,40	0
2	NLT	E	404	26/26	0.67	0.43	1.47	38,40,41,41	0
2	NLT	F	405	26/26	0.72	0.43	1.36	39,40,42,42	0
2	NLT	C	402	26/26	0.69	0.45	0.95	38,40,41,41	0
2	NLT	A	400	26/26	0.73	0.36	0.45	39,40,41,42	0
2	NLT	H	407	26/26	0.73	0.38	0.42	39,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.