



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:27 am BST

PDB ID : 6BUH
Title : Crystal structure of a membrane protein, crystal form II
Authors : Ma, D.; Wang, Z.; Xu, W.
Deposited on : 2017-12-10
Resolution : 3.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

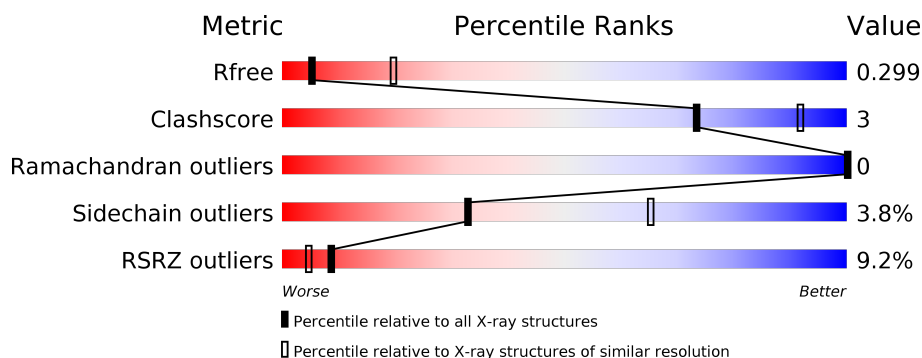
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 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	82	<div> <div>35%</div> <div> <div>84%</div> <div>12%</div> <div>•</div> </div> </div>
1	B	82	<div> <div>20%</div> <div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>
1	E	82	<div> <div>35%</div> <div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>
1	G	82	<div> <div>52%</div> <div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>
2	C	425	<div> <div>2%</div> <div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>
2	D	425	<div> <div>4%</div> <div> <div>84%</div> <div>13%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	425	<div><div></div><div>3%</div><div>84%</div><div>13%</div><div></div></div>
2	H	425	<div><div></div><div>6%</div><div>84%</div><div>13%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16308 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 D-alanyl carrier protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	P	S	0	0	0
			629	390	97	136	1	5			
1	B	79	Total	C	N	O	P	S	0	0	0
			629	390	97	136	1	5			
1	E	79	Total	C	N	O	P	S	0	0	0
			629	390	97	136	1	5			
1	G	79	Total	C	N	O	P	S	0	0	0
			629	390	97	136	1	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5M0A6
A	-1	SER	-	expression tag	UNP Q5M0A6
A	0	HIS	-	expression tag	UNP Q5M0A6
B	-2	GLY	-	expression tag	UNP Q5M0A6
B	-1	SER	-	expression tag	UNP Q5M0A6
B	0	HIS	-	expression tag	UNP Q5M0A6
E	-2	GLY	-	expression tag	UNP Q5M0A6
E	-1	SER	-	expression tag	UNP Q5M0A6
E	0	HIS	-	expression tag	UNP Q5M0A6
G	-2	GLY	-	expression tag	UNP Q5M0A6
G	-1	SER	-	expression tag	UNP Q5M0A6
G	0	HIS	-	expression tag	UNP Q5M0A6

- Molecule 2 is a protein called D-alanyl transfer protein DltB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	414	Total	C	N	O	S		0	0	0
			3448	2327	548	553	20				
2	D	414	Total	C	N	O	S		0	0	0
			3448	2327	548	553	20				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	414	Total	C	N	O	S	0	0	0
			3448	2327	548	553	20			
2	H	414	Total	C	N	O	S	0	0	0
			3448	2327	548	553	20			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	416	LEU	-	expression tag	UNP Q5M4V4
C	417	GLU	-	expression tag	UNP Q5M4V4
C	418	HIS	-	expression tag	UNP Q5M4V4
C	419	HIS	-	expression tag	UNP Q5M4V4
C	420	HIS	-	expression tag	UNP Q5M4V4
C	421	HIS	-	expression tag	UNP Q5M4V4
C	422	HIS	-	expression tag	UNP Q5M4V4
C	423	HIS	-	expression tag	UNP Q5M4V4
C	424	HIS	-	expression tag	UNP Q5M4V4
C	425	HIS	-	expression tag	UNP Q5M4V4
D	416	LEU	-	expression tag	UNP Q5M4V4
D	417	GLU	-	expression tag	UNP Q5M4V4
D	418	HIS	-	expression tag	UNP Q5M4V4
D	419	HIS	-	expression tag	UNP Q5M4V4
D	420	HIS	-	expression tag	UNP Q5M4V4
D	421	HIS	-	expression tag	UNP Q5M4V4
D	422	HIS	-	expression tag	UNP Q5M4V4
D	423	HIS	-	expression tag	UNP Q5M4V4
D	424	HIS	-	expression tag	UNP Q5M4V4
D	425	HIS	-	expression tag	UNP Q5M4V4
F	416	LEU	-	expression tag	UNP Q5M4V4
F	417	GLU	-	expression tag	UNP Q5M4V4
F	418	HIS	-	expression tag	UNP Q5M4V4
F	419	HIS	-	expression tag	UNP Q5M4V4
F	420	HIS	-	expression tag	UNP Q5M4V4
F	421	HIS	-	expression tag	UNP Q5M4V4
F	422	HIS	-	expression tag	UNP Q5M4V4
F	423	HIS	-	expression tag	UNP Q5M4V4
F	424	HIS	-	expression tag	UNP Q5M4V4
F	425	HIS	-	expression tag	UNP Q5M4V4
H	416	LEU	-	expression tag	UNP Q5M4V4
H	417	GLU	-	expression tag	UNP Q5M4V4
H	418	HIS	-	expression tag	UNP Q5M4V4
H	419	HIS	-	expression tag	UNP Q5M4V4

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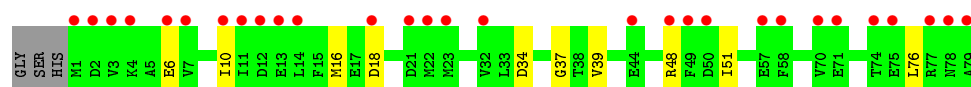
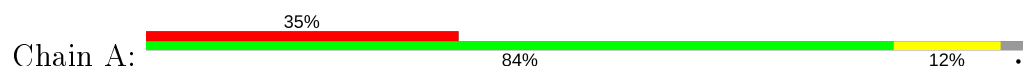
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Chain	Residue	Modelled	Actual	Comment	Reference
H	420	HIS	-	expression tag	UNP Q5M4V4
H	421	HIS	-	expression tag	UNP Q5M4V4
H	422	HIS	-	expression tag	UNP Q5M4V4
H	423	HIS	-	expression tag	UNP Q5M4V4
H	424	HIS	-	expression tag	UNP Q5M4V4
H	425	HIS	-	expression tag	UNP Q5M4V4

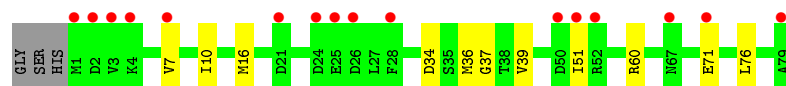
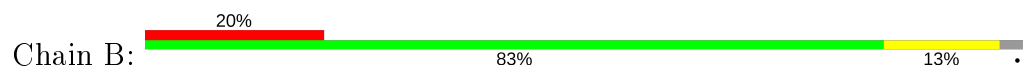
3 Residue-property plots [i](#)

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

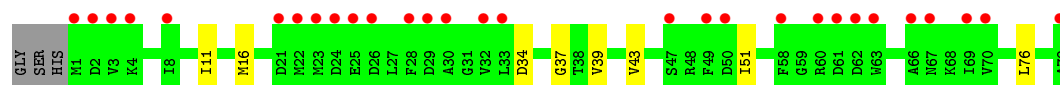
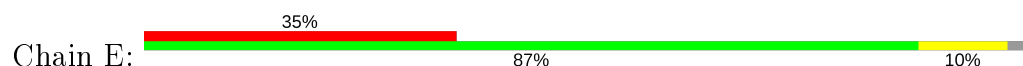
- Molecule 1: D-alanyl carrier protein



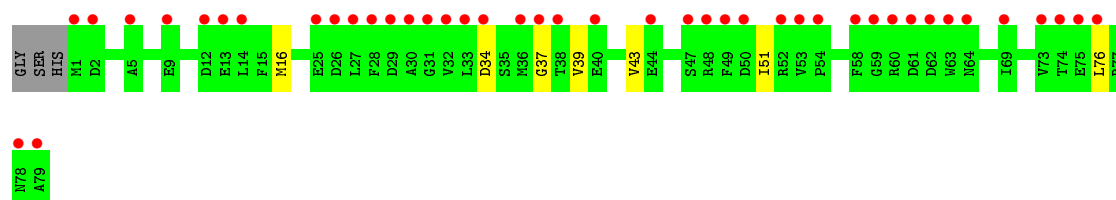
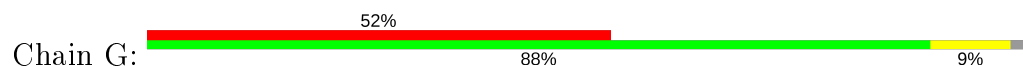
- Molecule 1: D-alanyl carrier protein



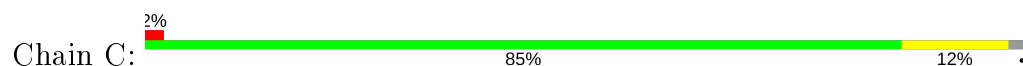
- Molecule 1: D-alanyl carrier protein

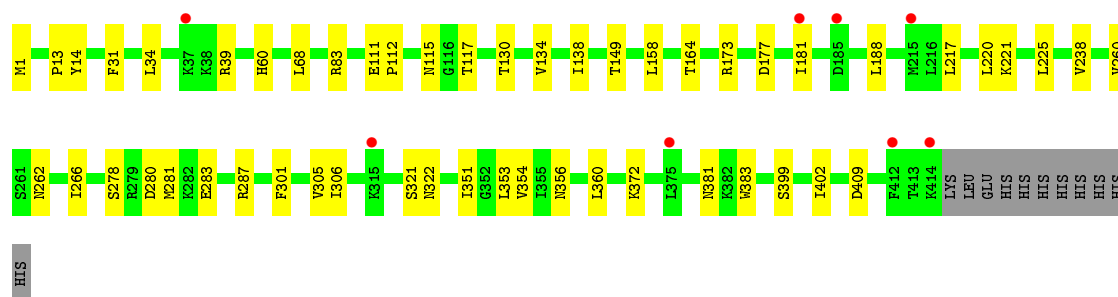


- Molecule 1: D-alanyl carrier protein

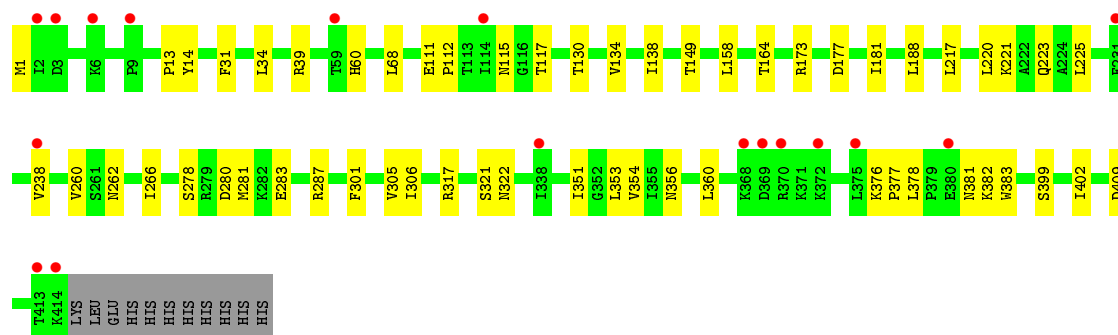
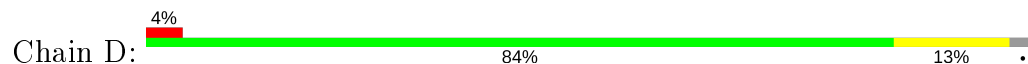


- Molecule 2: D-alanyl transfer protein DltB

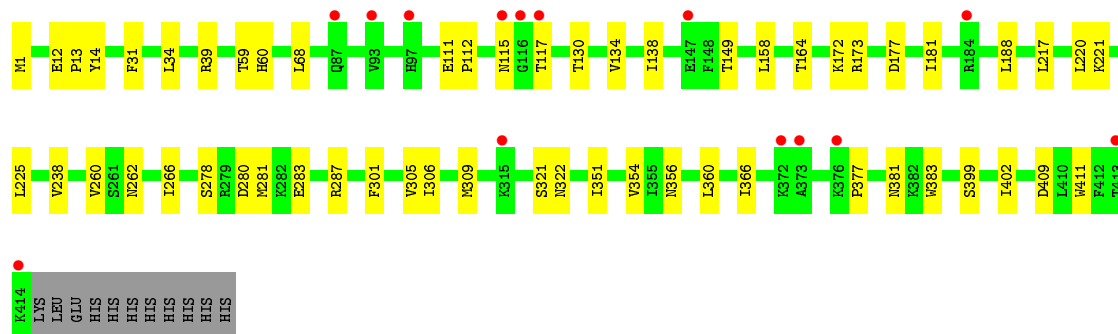
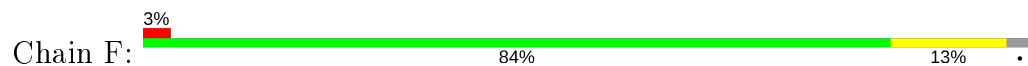




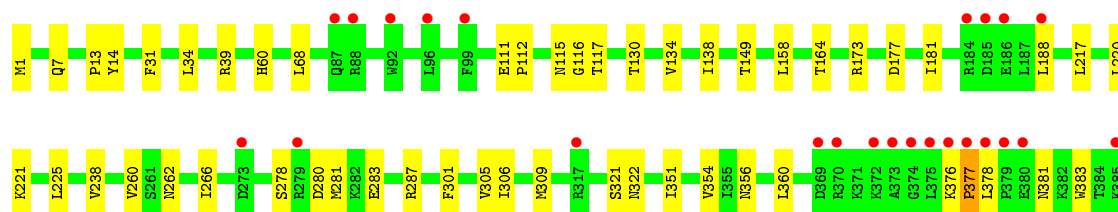
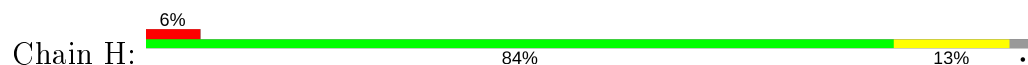
• Molecule 2: D-alanyl transfer protein DltB

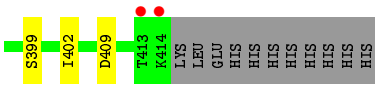


• Molecule 2: D-alanyl transfer protein DltB



• Molecule 2: D-alanyl transfer protein DltB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.68Å 124.58Å 126.71Å 90.00° 96.99° 90.00°	Depositor
Resolution (Å)	125.77 – 3.15 48.52 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (125.77-3.15) 98.3 (48.52-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.276 , 0.299 0.277 , 0.299	Depositor DCC
R_{free} test set	2832 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16308	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/624	0.65	0/841
1	B	0.44	0/624	0.66	0/841
1	E	0.44	0/624	0.68	0/841
1	G	0.45	0/624	0.66	0/841
2	C	0.48	0/3556	0.65	0/4811
2	D	0.47	0/3556	0.64	0/4811
2	F	0.47	0/3556	0.64	0/4811
2	H	0.47	0/3556	0.64	0/4811
All	All	0.47	0/16720	0.65	0/22608

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	629	0	600	4	0
1	B	629	0	600	7	0
1	E	629	0	600	5	0
1	G	629	0	600	4	0
2	C	3448	0	3527	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3448	0	3527	26	0
2	F	3448	0	3527	27	0
2	H	3448	0	3527	26	0
All	All	16308	0	16508	107	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 3.

All (107) 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:71:GLU:HG3	2:H:116:GLY:HA3	1.58	0.85
2:H:280:ASP:HB3	2:H:283:GLU:H	1.63	0.64
2:C:280:ASP:HB3	2:C:283:GLU:H	1.62	0.64
2:D:130:THR:O	2:D:134:VAL:HG23	1.98	0.64
2:F:280:ASP:HB3	2:F:283:GLU:H	1.63	0.64
2:D:280:ASP:HB3	2:D:283:GLU:H	1.62	0.63
2:F:130:THR:O	2:F:134:VAL:HG23	1.98	0.63
2:C:130:THR:O	2:C:134:VAL:HG23	1.99	0.63
2:H:130:THR:O	2:H:134:VAL:HG23	1.98	0.62
1:A:39:VAL:HG13	2:C:306:ILE:HD13	1.82	0.61
1:E:39:VAL:HG13	2:F:306:ILE:HD13	1.85	0.59
2:D:381:ASN:HD22	2:D:383:TRP:H	1.53	0.56
2:F:381:ASN:HD22	2:F:383:TRP:H	1.54	0.56
2:D:217:LEU:HG	2:D:221:LYS:HD2	1.88	0.56
2:H:13:PRO:HG3	2:H:164:THR:HG21	1.86	0.56
2:C:381:ASN:HD22	2:C:383:TRP:H	1.53	0.55
1:A:10:ILE:HD13	1:A:48:ARG:HD2	1.87	0.55
2:H:381:ASN:HD22	2:H:383:TRP:H	1.54	0.55
2:F:13:PRO:HG3	2:F:164:THR:HG21	1.88	0.55
2:C:217:LEU:HG	2:C:221:LYS:HD2	1.88	0.55
2:F:217:LEU:HG	2:F:221:LYS:HD2	1.89	0.54
1:A:34:ASP:HB2	1:A:37:GLY:H	1.73	0.54
2:H:217:LEU:HG	2:H:221:LYS:HD2	1.89	0.54
2:D:13:PRO:HG3	2:D:164:THR:HG21	1.89	0.54
1:B:39:VAL:HG13	2:D:306:ILE:HD13	1.89	0.54
2:D:383:TRP:CZ2	2:F:411:TRP:HB3	2.43	0.54
2:H:376:LYS:HG3	2:H:377:PRO:HD2	1.89	0.54
1:B:34:ASP:HB2	1:B:37:GLY:H	1.74	0.53
2:D:301:PHE:O	2:D:305:VAL:HG23	2.08	0.53
2:C:301:PHE:O	2:C:305:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:301:PHE:O	2:F:305:VAL:HG23	2.09	0.52
2:H:301:PHE:O	2:H:305:VAL:HG23	2.08	0.52
1:E:34:ASP:HB2	1:E:37:GLY:H	1.74	0.52
1:G:34:ASP:HB2	1:G:37:GLY:H	1.75	0.52
2:D:115:ASN:HB3	2:D:117:THR:H	1.75	0.51
2:C:115:ASN:HB3	2:C:117:THR:H	1.76	0.51
2:F:399:SER:HA	2:F:402:ILE:HD12	1.93	0.51
2:F:115:ASN:HB3	2:F:117:THR:H	1.75	0.50
2:H:115:ASN:HB3	2:H:117:THR:H	1.76	0.50
2:H:399:SER:HA	2:H:402:ILE:HD12	1.93	0.50
2:C:83:ARG:HG2	2:H:7:GLN:HE21	1.77	0.50
2:D:399:SER:HA	2:D:402:ILE:HD12	1.93	0.49
2:C:13:PRO:HG3	2:C:164:THR:HG21	1.93	0.49
2:C:399:SER:HA	2:C:402:ILE:HD12	1.93	0.49
1:E:43:VAL:HG21	2:F:309:MET:HB3	1.94	0.49
2:D:383:TRP:HZ2	2:F:411:TRP:HB3	1.77	0.48
2:D:220:LEU:HB3	2:D:238:VAL:HG12	1.96	0.48
2:D:31:PHE:HA	2:D:34:LEU:HD12	1.96	0.48
2:H:220:LEU:HB3	2:H:238:VAL:HG12	1.96	0.48
2:F:220:LEU:HB3	2:F:238:VAL:HG12	1.96	0.48
2:H:31:PHE:HA	2:H:34:LEU:HD12	1.96	0.47
2:F:31:PHE:HA	2:F:34:LEU:HD12	1.95	0.47
2:C:31:PHE:HA	2:C:34:LEU:HD12	1.95	0.47
1:B:36:MET:HG2	2:D:317:ARG:HG2	1.96	0.47
1:B:71:GLU:CG	2:H:116:GLY:HA3	2.35	0.47
2:C:220:LEU:HB3	2:C:238:VAL:HG12	1.97	0.47
2:D:376:LYS:HG2	2:D:377:PRO:HD2	1.95	0.47
2:D:225:LEU:HD21	2:D:409:ASP:HB3	1.98	0.46
2:F:280:ASP:HB3	2:F:283:GLU:HB2	1.97	0.46
2:F:134:VAL:O	2:F:138:ILE:HG12	2.15	0.46
2:C:14:TYR:HE1	2:C:260:VAL:HG21	1.80	0.46
2:H:134:VAL:O	2:H:138:ILE:HG12	2.15	0.46
2:F:14:TYR:HE1	2:F:260:VAL:HG21	1.80	0.46
2:F:278:SER:HB3	2:F:287:ARG:HD2	1.98	0.46
2:H:280:ASP:HB3	2:H:283:GLU:HB2	1.98	0.46
2:C:278:SER:HB3	2:C:287:ARG:HD2	1.97	0.46
2:C:225:LEU:HD21	2:C:409:ASP:HB3	1.98	0.46
1:E:51:ILE:HG21	1:E:76:LEU:HB3	1.98	0.46
2:H:278:SER:HB3	2:H:287:ARG:HD2	1.97	0.46
2:D:134:VAL:O	2:D:138:ILE:HG12	2.15	0.46
1:B:51:ILE:HG21	1:B:76:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:VAL:O	2:C:138:ILE:HG12	2.15	0.45
2:D:14:TYR:HE1	2:D:260:VAL:HG21	1.80	0.45
2:F:351:ILE:HA	2:F:354:VAL:HG22	1.97	0.45
2:H:14:TYR:HE1	2:H:260:VAL:HG21	1.81	0.45
2:C:280:ASP:HB3	2:C:283:GLU:HB2	1.98	0.45
2:C:372:LYS:HE2	2:F:59:THR:HB	1.98	0.45
1:E:39:VAL:HG11	2:F:305:VAL:HG12	1.99	0.45
1:A:51:ILE:HG21	1:A:76:LEU:HB3	1.98	0.45
1:G:51:ILE:HG21	1:G:76:LEU:HB3	1.99	0.45
2:D:280:ASP:HB3	2:D:283:GLU:HB2	1.98	0.45
2:D:278:SER:HB3	2:D:287:ARG:HD2	1.98	0.44
2:C:83:ARG:HG2	2:H:7:GLN:NE2	2.32	0.44
2:F:39:ARG:HG3	2:F:181:ILE:HD11	2.00	0.44
2:D:281:MET:HB3	2:D:353:LEU:HD12	2.00	0.44
2:F:225:LEU:HD21	2:F:409:ASP:HB3	1.98	0.44
2:H:39:ARG:HG3	2:H:181:ILE:HD11	2.00	0.44
2:H:351:ILE:HA	2:H:354:VAL:HG22	1.99	0.43
2:C:111:GLU:HB3	2:C:112:PRO:HD3	2.01	0.43
2:H:225:LEU:HD21	2:H:409:ASP:HB3	2.00	0.43
2:C:372:LYS:HB3	2:F:59:THR:HB	2.00	0.43
2:D:351:ILE:HA	2:D:354:VAL:HG22	2.00	0.42
2:D:281:MET:H	2:D:356:ASN:ND2	2.17	0.42
2:C:351:ILE:HA	2:C:354:VAL:HG22	2.00	0.42
1:G:39:VAL:HG13	2:H:306:ILE:HD13	2.01	0.42
2:C:39:ARG:HG3	2:C:181:ILE:HD11	2.01	0.42
2:H:281:MET:H	2:H:356:ASN:ND2	2.18	0.42
2:D:223:GLN:OE1	2:F:366:ILE:HG12	2.19	0.42
2:D:111:GLU:HB3	2:D:112:PRO:HD3	2.01	0.42
2:C:281:MET:HB3	2:C:353:LEU:HD12	2.00	0.42
2:F:281:MET:H	2:F:356:ASN:ND2	2.18	0.42
1:G:43:VAL:HG21	2:H:309:MET:HB3	2.03	0.41
2:C:281:MET:H	2:C:356:ASN:ND2	2.18	0.41
2:D:39:ARG:HG3	2:D:181:ILE:HD11	2.00	0.41
2:F:111:GLU:HB3	2:F:112:PRO:HD3	2.02	0.40
1:B:7:VAL:HA	1:B:10:ILE:HG22	2.04	0.40
2:H:111:GLU:HB3	2:H:112:PRO:HD3	2.02	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	76/82 (93%)	70 (92%)	6 (8%)	0	100	100
1	B	76/82 (93%)	70 (92%)	6 (8%)	0	100	100
1	E	76/82 (93%)	70 (92%)	6 (8%)	0	100	100
1	G	76/82 (93%)	70 (92%)	6 (8%)	0	100	100
2	C	412/425 (97%)	393 (95%)	19 (5%)	0	100	100
2	D	412/425 (97%)	393 (95%)	19 (5%)	0	100	100
2	F	412/425 (97%)	393 (95%)	19 (5%)	0	100	100
2	H	412/425 (97%)	392 (95%)	20 (5%)	0	100	100
All	All	1952/2028 (96%)	1851 (95%)	101 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	70/72 (97%)	67 (96%)	3 (4%)	29	62
1	B	70/72 (97%)	68 (97%)	2 (3%)	42	72
1	E	70/72 (97%)	68 (97%)	2 (3%)	42	72
1	G	70/72 (97%)	69 (99%)	1 (1%)	67	85
2	C	370/381 (97%)	357 (96%)	13 (4%)	36	67
2	D	370/381 (97%)	355 (96%)	15 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	370/381 (97%)	354 (96%)	16 (4%)	29	62
2	H	370/381 (97%)	355 (96%)	15 (4%)	30	63
All	All	1760/1812 (97%)	1693 (96%)	67 (4%)	33	65

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	16	MET
1	A	18	ASP
2	C	1	MET
2	C	60	HIS
2	C	68	LEU
2	C	149	THR
2	C	158	LEU
2	C	173	ARG
2	C	177	ASP
2	C	188	LEU
2	C	262	ASN
2	C	266	ILE
2	C	321	SER
2	C	322	ASN
2	C	360	LEU
1	B	16	MET
1	B	60	ARG
2	D	1	MET
2	D	60	HIS
2	D	68	LEU
2	D	149	THR
2	D	158	LEU
2	D	173	ARG
2	D	177	ASP
2	D	188	LEU
2	D	262	ASN
2	D	266	ILE
2	D	321	SER
2	D	322	ASN
2	D	360	LEU
2	D	378	LEU
2	D	382	LYS
1	E	11	ILE

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Mol	Chain	Res	Type
1	E	16	MET
2	F	1	MET
2	F	12	GLU
2	F	60	HIS
2	F	68	LEU
2	F	149	THR
2	F	158	LEU
2	F	172	LYS
2	F	173	ARG
2	F	177	ASP
2	F	188	LEU
2	F	262	ASN
2	F	266	ILE
2	F	321	SER
2	F	322	ASN
2	F	360	LEU
2	F	377	PRO
1	G	16	MET
2	H	1	MET
2	H	60	HIS
2	H	68	LEU
2	H	149	THR
2	H	158	LEU
2	H	173	ARG
2	H	177	ASP
2	H	188	LEU
2	H	262	ASN
2	H	266	ILE
2	H	321	SER
2	H	322	ASN
2	H	360	LEU
2	H	377	PRO
2	H	378	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
2	C	90	ASN
2	C	115	ASN
2	C	183	ASN
2	C	381	ASN

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Mol	Chain	Res	Type
2	C	394	ASN
1	B	67	ASN
2	D	90	ASN
2	D	115	ASN
2	D	183	ASN
2	D	381	ASN
2	D	394	ASN
1	E	67	ASN
2	F	10	HIS
2	F	90	ASN
2	F	115	ASN
2	F	183	ASN
2	F	381	ASN
2	F	394	ASN
2	H	7	GLN
2	H	90	ASN
2	H	115	ASN
2	H	183	ASN
2	H	381	ASN
2	H	394	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	E	35	1	8,9,10	0.60	0	8,12,14	1.70	2 (25%)
1	SEP	B	35	1	8,9,10	0.64	0	8,12,14	1.54	1 (12%)
1	SEP	A	35	1	8,9,10	0.64	0	8,12,14	1.36	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	G	35	1	8,9,10	0.67	0	8,12,14	1.58	1 (12%)

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
1	SEP	E	35	1	-	5/5/8/10	-
1	SEP	B	35	1	-	5/5/8/10	-
1	SEP	A	35	1	-	5/5/8/10	-
1	SEP	G	35	1	-	5/5/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	SEP	OG-CB-CA	3.07	111.13	108.14
1	G	35	SEP	OG-CB-CA	3.01	111.08	108.14
1	B	35	SEP	OG-CB-CA	2.87	110.94	108.14
1	A	35	SEP	OG-CB-CA	2.50	110.58	108.14
1	E	35	SEP	P-OG-CB	2.04	123.91	118.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	35	SEP	N-CA-CB-OG
1	E	35	SEP	CB-OG-P-O2P
1	E	35	SEP	CB-OG-P-O3P
1	B	35	SEP	N-CA-CB-OG
1	B	35	SEP	CB-OG-P-O2P
1	B	35	SEP	CB-OG-P-O3P
1	A	35	SEP	N-CA-CB-OG
1	A	35	SEP	CB-OG-P-O2P
1	A	35	SEP	CB-OG-P-O3P
1	G	35	SEP	N-CA-CB-OG
1	G	35	SEP	CB-OG-P-O2P
1	G	35	SEP	CB-OG-P-O3P
1	E	35	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
1	B	35	SEP	CB-OG-P-O1P
1	A	35	SEP	CB-OG-P-O1P
1	G	35	SEP	CB-OG-P-O1P
1	E	35	SEP	CA-CB-OG-P
1	B	35	SEP	CA-CB-OG-P
1	A	35	SEP	CA-CB-OG-P
1	G	35	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	78/82 (95%)	1.99	29 (37%) 0 0	138, 170, 188, 208	1 (1%)
1	B	78/82 (95%)	1.00	16 (20%) 1 0	110, 142, 164, 173	1 (1%)
1	E	78/82 (95%)	1.62	29 (37%) 0 0	100, 131, 163, 168	1 (1%)
1	G	78/82 (95%)	2.67	43 (55%) 0 0	160, 189, 207, 211	1 (1%)
2	C	414/425 (97%)	0.03	8 (1%) 66 53	53, 74, 102, 156	0
2	D	414/425 (97%)	0.11	17 (4%) 37 22	57, 76, 126, 166	0
2	F	414/425 (97%)	0.12	14 (3%) 45 28	54, 80, 115, 144	0
2	H	414/425 (97%)	0.35	26 (6%) 20 10	64, 93, 142, 169	0
All	All	1968/2028 (97%)	0.42	182 (9%) 9 5	53, 84, 174, 211	4 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	THR	12.1
1	A	78	ASN	10.7
2	H	374	GLY	10.6
1	G	75	GLU	10.1
1	G	79	ALA	9.8
1	A	1	MET	8.5
1	G	13	GLU	8.4
1	A	77	ARG	7.9
1	E	50	ASP	7.8
1	G	29	ASP	7.4
1	G	63	TRP	7.3
1	A	75	GLU	7.1
2	H	373	ALA	7.0
1	G	26	ASP	7.0
2	D	372	LYS	6.9
1	G	1	MET	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	49	PHE	6.8
1	A	7	VAL	6.4
2	H	380	GLU	6.1
2	H	379	PRO	6.1
2	H	375	LEU	6.0
1	A	3	VAL	5.9
1	A	21	ASP	5.7
1	E	1	MET	5.7
1	E	61	ASP	5.5
1	B	25	GLU	5.4
2	H	185	ASP	5.4
1	G	27	LEU	5.3
1	G	64	ASN	5.3
1	G	34	ASP	5.2
1	A	58	PHE	5.1
1	A	13	GLU	5.1
1	E	62	ASP	5.0
1	B	1	MET	5.0
1	B	28	PHE	5.0
1	G	28	PHE	4.8
1	G	62	ASP	4.8
2	H	279	ARG	4.7
1	B	3	VAL	4.7
1	E	79	ALA	4.7
1	G	52	ARG	4.6
1	G	9	GLU	4.6
1	E	60	ARG	4.5
2	H	372	LYS	4.5
1	G	33	LEU	4.5
1	G	32	VAL	4.5
1	E	28	PHE	4.4
1	G	40	GLU	4.4
1	E	21	ASP	4.3
1	G	50	ASP	4.3
1	A	50	ASP	4.3
2	D	3	ASP	4.3
1	E	63	TRP	4.3
1	A	10	ILE	4.3
1	A	79	ALA	4.2
1	A	12	ASP	4.2
1	B	4	LYS	4.2
2	H	369	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	2	ASP	4.1
1	B	79	ALA	4.1
1	B	2	ASP	4.1
1	G	61	ASP	4.0
1	E	32	VAL	3.9
2	F	115	ASN	3.9
2	D	413	THR	3.9
1	A	23	MET	3.9
1	G	48	ARG	3.8
2	C	185	ASP	3.8
2	D	414	LYS	3.8
1	A	71	GLU	3.7
2	D	114	ILE	3.7
2	H	378	LEU	3.7
1	E	70	VAL	3.7
1	A	32	VAL	3.7
1	E	33	LEU	3.7
1	A	22	MET	3.6
2	D	338	ILE	3.5
1	G	78	ASN	3.5
1	A	48	ARG	3.4
1	G	49	PHE	3.4
1	G	76	LEU	3.4
2	D	2	ILE	3.3
2	C	414	LYS	3.2
1	E	25	GLU	3.2
1	E	58	PHE	3.2
2	H	92	TRP	3.2
2	H	188	LEU	3.2
1	E	66	ALA	3.2
1	E	24	ASP	3.2
2	F	414	LYS	3.1
2	F	315	LYS	3.1
1	G	73	VAL	3.1
2	H	385	LYS	3.1
1	G	60	ARG	3.1
1	G	12	ASP	3.1
1	G	36	MET	3.1
2	D	6	LYS	3.1
2	H	370	ARG	3.1
2	D	375	LEU	3.1
1	E	2	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	58	PHE	3.0
1	G	30	ALA	3.0
1	G	31	GLY	2.9
2	F	93	VAL	2.9
2	H	273	ASP	2.9
2	D	370	ARG	2.9
1	G	54	PRO	2.9
1	B	24	ASP	2.8
2	F	147	GLU	2.8
1	G	38	THR	2.8
2	F	372	LYS	2.8
2	D	59	THR	2.8
1	G	2	ASP	2.8
1	E	30	ALA	2.7
2	H	87	GLN	2.7
2	C	315	LYS	2.7
1	E	3	VAL	2.7
1	G	44	GLU	2.6
2	C	181	ILE	2.6
1	A	44	GLU	2.6
1	G	53	VAL	2.6
1	G	14	LEU	2.6
2	H	186	GLU	2.6
2	F	184	ARG	2.6
2	C	37	LYS	2.6
1	G	74	THR	2.5
1	A	6	GLU	2.5
1	A	11	ILE	2.5
1	B	71	GLU	2.5
1	A	14	LEU	2.5
2	D	369	ASP	2.5
1	A	4	LYS	2.5
2	D	368	LYS	2.5
1	G	37	GLY	2.5
1	B	21	ASP	2.5
1	E	22	MET	2.5
1	G	25	GLU	2.5
1	E	49	PHE	2.5
2	H	414	LYS	2.5
2	F	373	ALA	2.5
2	H	377	PRO	2.4
1	A	57	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	50	ASP	2.4
1	E	47	SER	2.4
1	E	4	LYS	2.4
1	G	59	GLY	2.4
2	C	412	PHE	2.3
1	G	5	ALA	2.3
1	A	70	VAL	2.3
1	G	47	SER	2.3
2	F	97	HIS	2.3
2	H	317	ARG	2.3
2	C	375	LEU	2.3
2	H	376	LYS	2.3
1	E	67	ASN	2.3
1	B	26	ASP	2.2
1	E	23	MET	2.2
2	D	9	PRO	2.2
1	E	26	ASP	2.2
2	C	215	MET	2.2
1	E	29	ASP	2.2
2	F	117	THR	2.2
2	H	88	ARG	2.2
2	F	116	GLY	2.2
2	D	231	PHE	2.2
2	F	413	THR	2.2
1	B	7	VAL	2.1
1	G	69	ILE	2.1
1	B	67	ASN	2.1
2	H	99	PHE	2.1
2	F	376	LYS	2.1
1	E	69	ILE	2.1
2	H	413	THR	2.1
1	B	51	ILE	2.1
2	D	238	VAL	2.0
1	E	8	ILE	2.0
2	D	380	GLU	2.0
1	A	18	ASP	2.0
1	B	52	ARG	2.0
2	F	87	GLN	2.0
2	H	96	LEU	2.0
2	H	184	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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
1	SEP	G	35	10/11	0.71	0.27	182,183,184,186	0
1	SEP	A	35	10/11	0.83	0.21	163,167,171,174	0
1	SEP	E	35	10/11	0.85	0.20	129,141,146,151	0
1	SEP	B	35	10/11	0.91	0.21	129,132,137,143	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.