



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2017 – 02:18 PM EST

PDB ID : 6B9S  
Title : MPnS crystallized in the absence of substrate  
Authors : Born, D.A.; Drennan, C.L.  
Deposited on : unknown  
Resolution : 2.37 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](mailto: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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

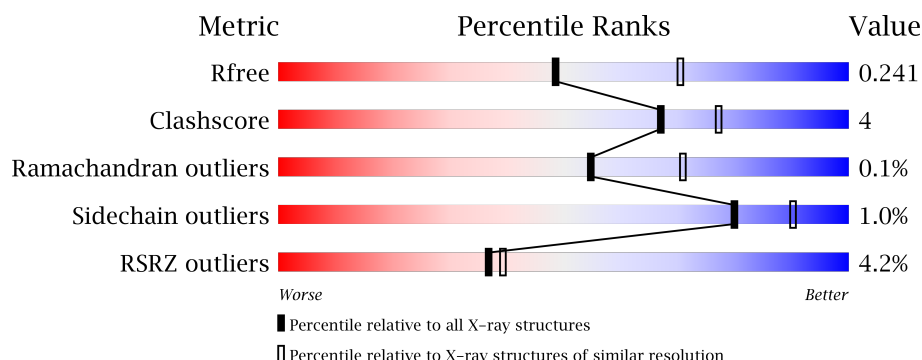
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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))
$R_{free}$	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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  $\geq 3$ , 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	457	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	B	457	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	C	457	<div> <div>6%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
1	D	457	<div> <div>4%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	E	457	<div> <div>7%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	457	
1	G	457	
1	H	457	

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	FE	C	501	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28405 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 Methylphosphonate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3482	2214	578	677	13			
1	D	441	Total	C	N	O	S	0	1	0
			3443	2191	573	666	13			
1	C	439	Total	C	N	O	S	0	0	0
			3407	2166	572	657	12			
1	F	397	Total	C	N	O	S	0	0	0
			3081	1961	512	596	12			
1	G	442	Total	C	N	O	S	0	0	0
			3443	2186	574	670	13			
1	B	441	Total	C	N	O	S	0	0	0
			3453	2193	578	669	13			
1	E	441	Total	C	N	O	S	0	0	0
			3405	2169	570	653	13			
1	H	429	Total	C	N	O	S	0	0	0
			3335	2121	557	646	11			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		

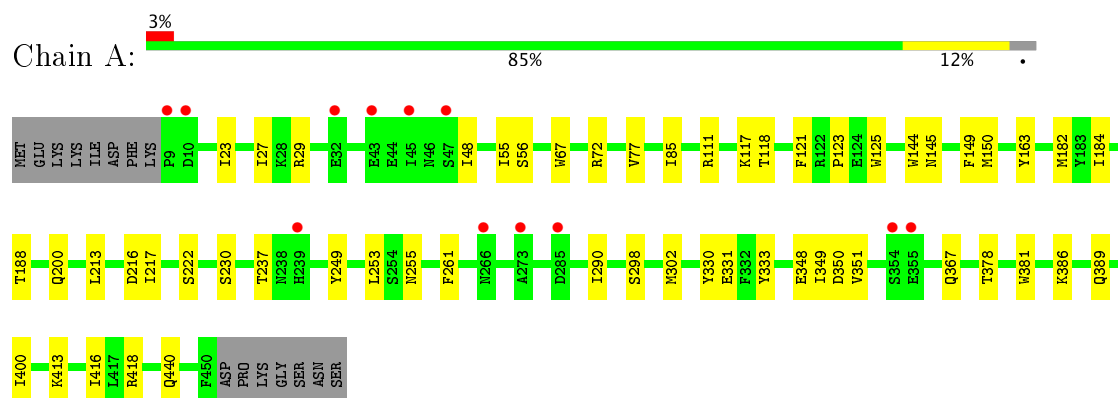
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	193	Total 193	O 193	0	0
3	D	222	Total 222	O 222	0	0
3	C	183	Total 183	O 183	0	0
3	F	136	Total 136	O 136	0	0
3	G	168	Total 168	O 168	0	0
3	B	157	Total 157	O 157	0	0
3	E	137	Total 137	O 137	0	0
3	H	155	Total 155	O 155	0	0

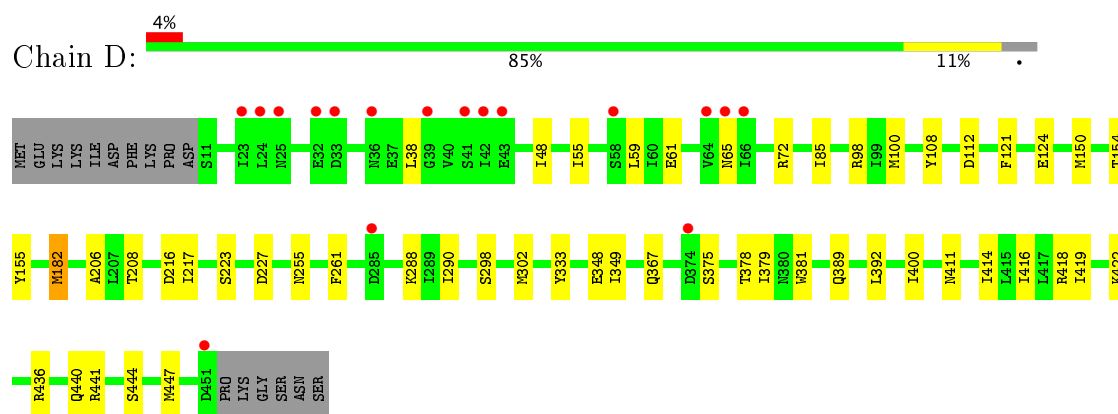
### 3 Residue-property plots [i](#)

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

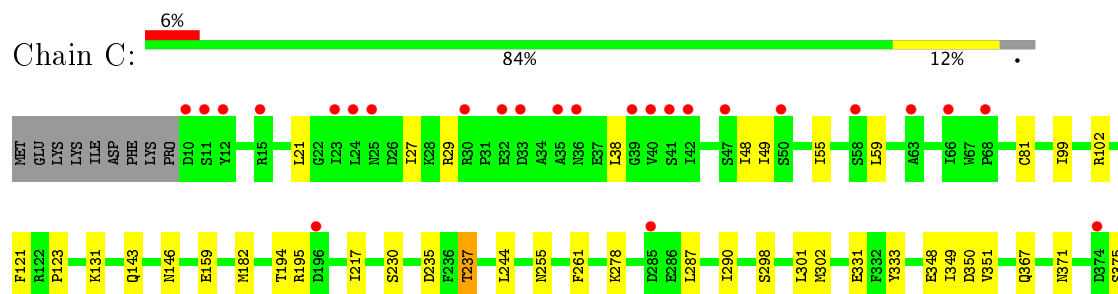
#### • Molecule 1: Methylphosphonate synthase



#### • Molecule 1: Methylphosphonate synthase

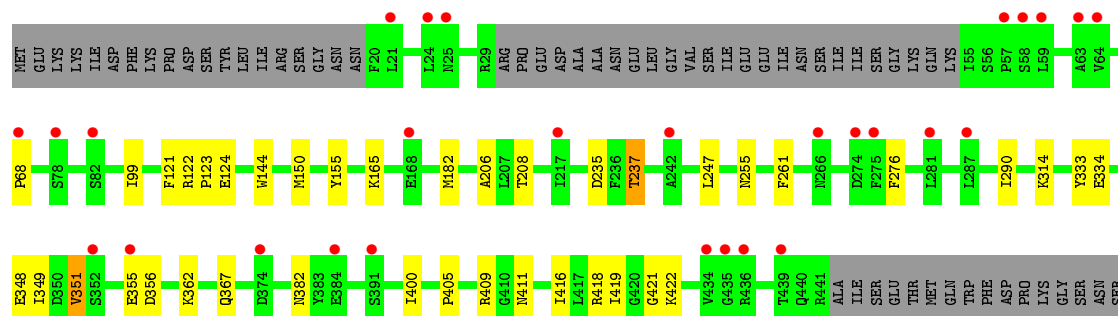
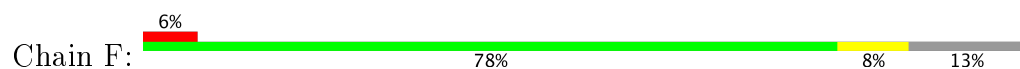


#### • Molecule 1: Methylphosphonate synthase

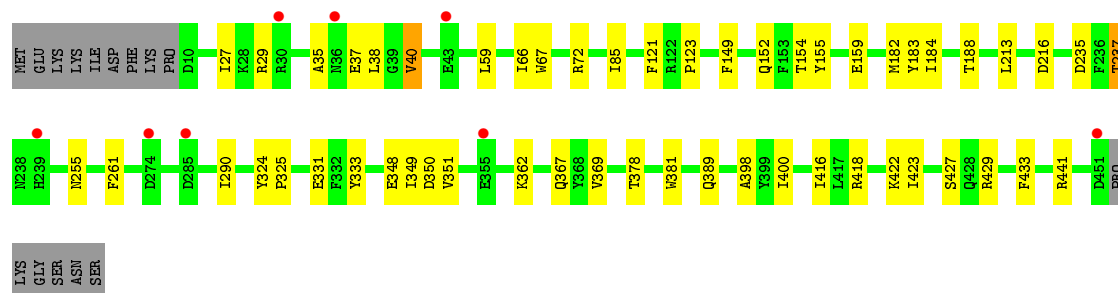
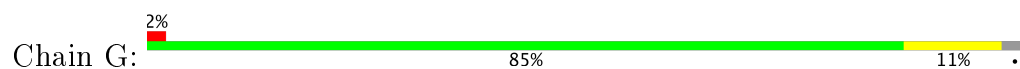




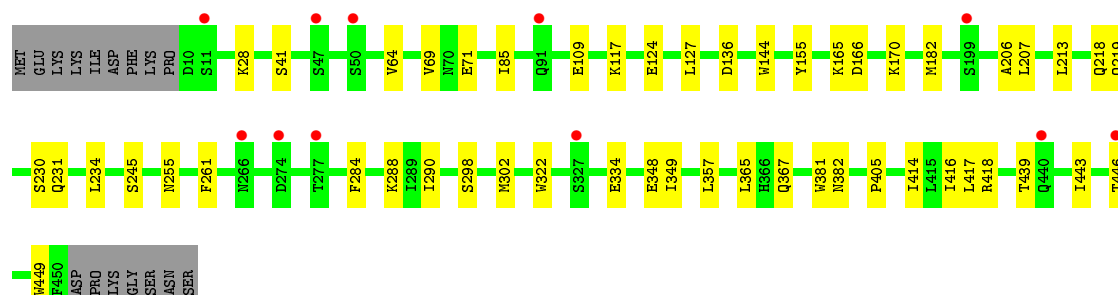
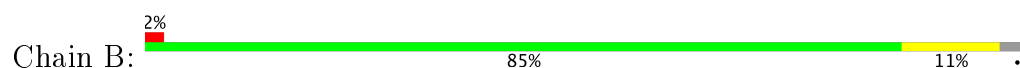
• Molecule 1: Methylphosphonate synthase



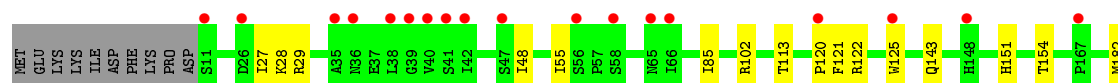
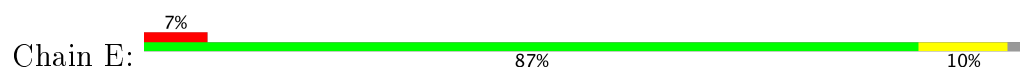
• Molecule 1: Methylphosphonate synthase

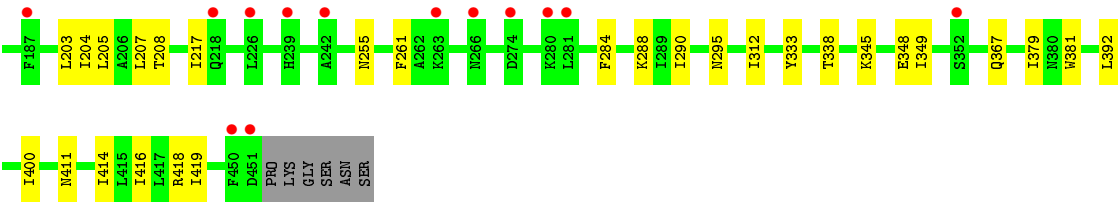


• Molecule 1: Methylphosphonate synthase

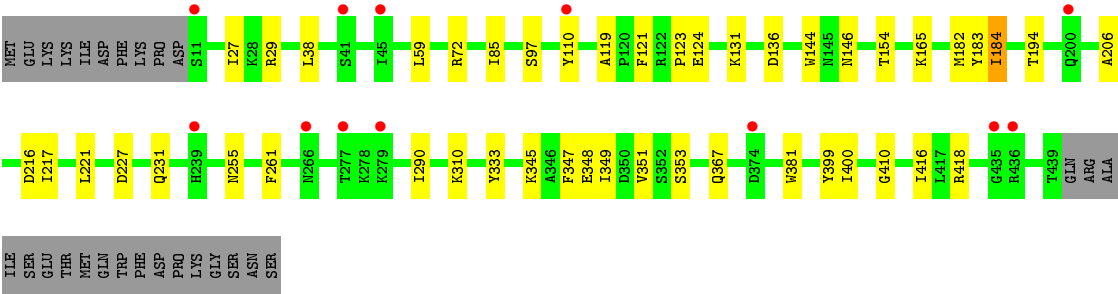
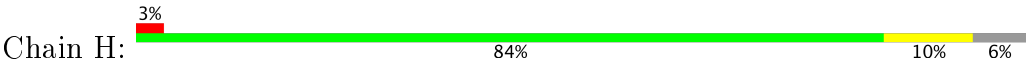


• Molecule 1: Methylphosphonate synthase





● Molecule 1: Methylphosphonate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	352.38Å 53.17Å 260.12Å 90.00° 122.34° 90.00°	Depositor
Resolution (Å)	10.03 – 2.37 10.03 – 2.37	Depositor EDS
% Data completeness (in resolution range)	97.6 (10.03-2.37) 97.6 (10.03-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.38Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.203 , 0.241 0.203 , 0.241	Depositor DCC
$R_{free}$ test set	7919 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FE

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	0.28	0/3565	0.48	1/4839 (0.0%)
1	B	0.26	0/3535	0.43	0/4803
1	C	0.27	0/3486	0.46	0/4738
1	D	0.28	0/3526	0.46	0/4791
1	E	0.27	0/3487	0.45	0/4743
1	F	0.26	0/3157	0.46	0/4292
1	G	0.27	0/3525	0.45	0/4792
1	H	0.26	0/3414	0.44	0/4641
All	All	0.27	0/27695	0.45	1/37639 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	THR	C-N-CA	6.33	137.53	121.70

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	3482	0	3310	34	0
1	B	3453	0	3268	32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3407	0	3212	36	0
1	D	3443	0	3234	33	0
1	E	3405	0	3182	31	0
1	F	3081	0	2847	26	0
1	G	3443	0	3231	36	0
1	H	3335	0	3136	30	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	193	0	0	3	1
3	B	157	0	0	2	0
3	C	183	0	0	1	0
3	D	222	0	0	2	1
3	E	137	0	0	4	0
3	F	136	0	0	1	0
3	G	168	0	0	3	0
3	H	155	0	0	1	0
All	All	28405	0	25420	234	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 4.

All (234) 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:72:ARG:NH1	1:A:216:ASP:OD1	2.07	0.87
1:F:367:GLN:HG2	1:F:418:ARG:HG2	1.64	0.79
1:D:367:GLN:HG2	1:D:418:ARG:HG2	1.65	0.77
1:D:72:ARG:NH1	1:D:216:ASP:OD1	2.18	0.76
1:F:356:ASP:HB3	1:F:409:ARG:HE	1.53	0.74
1:A:367:GLN:HG2	1:A:418:ARG:HG2	1.68	0.74
1:H:333:TYR:HB2	1:H:348:GLU:HB3	1.70	0.73
1:G:367:GLN:HG2	1:G:418:ARG:HG2	1.70	0.72
1:G:441:ARG:NH1	1:H:146:ASN:O	2.24	0.70
1:G:182:MET:HE1	1:G:184:ILE:HB	1.72	0.70
1:H:182:MET:HE1	1:H:184:ILE:HG23	1.73	0.69
1:C:367:GLN:HG2	1:C:418:ARG:HG2	1.73	0.69
1:G:261:PHE:HZ	1:G:290:ILE:HG23	1.59	0.67
1:C:333:TYR:HB2	1:C:348:GLU:HB3	1.76	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:PHE:HZ	1:F:290:ILE:HG23	1.60	0.67
1:E:333:TYR:HB2	1:E:348:GLU:HB3	1.77	0.66
1:F:333:TYR:HB2	1:F:348:GLU:HB3	1.78	0.65
1:H:367:GLN:HG2	1:H:418:ARG:HG2	1.78	0.65
1:D:48:ILE:HD13	1:D:55:ILE:HG13	1.80	0.64
1:G:378:THR:HG21	1:G:389:GLN:HE21	1.63	0.63
1:D:333:TYR:HB2	1:D:348:GLU:HB3	1.79	0.63
1:C:27:ILE:O	1:C:29:ARG:NH1	2.32	0.62
1:C:287:LEU:HD21	1:C:301:LEU:HB2	1.82	0.61
1:C:235:ASP:OD1	1:C:237:THR:OG1	2.18	0.61
1:E:102:ARG:NH2	3:E:602:HOH:O	2.33	0.61
1:G:333:TYR:HB2	1:G:348:GLU:HB3	1.83	0.61
1:G:72:ARG:NH1	1:G:216:ASP:OD1	2.35	0.60
1:C:261:PHE:HZ	1:C:290:ILE:HG23	1.64	0.60
1:E:367:GLN:HG2	1:E:418:ARG:HG2	1.82	0.60
1:D:261:PHE:HZ	1:D:290:ILE:HG23	1.67	0.60
1:A:48:ILE:HD13	1:A:55:ILE:HG13	1.84	0.60
1:G:422:LYS:HB3	1:H:217:ILE:HG12	1.82	0.60
1:A:386:LYS:NZ	3:A:604:HOH:O	2.34	0.60
1:G:362:LYS:NZ	3:G:609:HOH:O	2.35	0.59
1:A:333:TYR:HB2	1:A:348:GLU:HB3	1.83	0.59
1:F:121:PHE:HD2	1:F:419:ILE:HD11	1.68	0.59
1:D:378:THR:HG21	1:D:389:GLN:HE21	1.68	0.58
1:B:367:GLN:HG2	1:B:418:ARG:HG2	1.84	0.58
1:G:155:TYR:OH	1:G:348:GLU:OE2	2.17	0.58
1:A:440:GLN:HG3	1:B:230:SER:HB3	1.85	0.57
1:E:367:GLN:HB2	1:E:400:ILE:HB	1.85	0.57
1:H:38:LEU:HD13	1:H:59:LEU:HD11	1.84	0.57
1:A:261:PHE:HZ	1:A:290:ILE:HG23	1.70	0.57
1:E:48:ILE:HD13	1:E:55:ILE:HG13	1.86	0.57
1:B:155:TYR:OH	1:B:348:GLU:OE2	2.15	0.57
1:F:235:ASP:OD1	1:F:237:THR:OG1	2.21	0.57
1:B:124:GLU:HB2	1:B:206:ALA:HB3	1.86	0.56
1:F:124:GLU:HB2	1:F:206:ALA:HB3	1.87	0.56
1:B:349:ILE:HD12	1:B:416:ILE:HG13	1.87	0.55
1:F:349:ILE:HD12	1:F:416:ILE:HG13	1.88	0.55
1:C:121:PHE:HD1	1:C:123:PRO:HD3	1.72	0.55
1:B:28:LYS:NZ	3:B:504:HOH:O	2.36	0.55
1:D:288:LYS:NZ	3:D:606:HOH:O	2.39	0.54
1:G:159:GLU:OE1	3:G:601:HOH:O	2.18	0.54
1:A:111:ARG:HB2	1:A:125:TRP:HB3	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLN:OE1	3:B:501:HOH:O	2.18	0.54
1:C:121:PHE:HD2	1:C:419:ILE:HD11	1.73	0.54
1:E:261:PHE:HZ	1:E:290:ILE:HG23	1.72	0.54
1:E:125:TRP:CH2	1:E:205:LEU:HD11	2.42	0.54
1:D:414:ILE:HD12	1:D:416:ILE:HD11	1.89	0.54
1:A:331:GLU:HB3	1:A:350:ASP:HB2	1.89	0.54
1:C:244:LEU:HD22	1:C:278:LYS:HG3	1.89	0.53
1:B:85:ILE:HD12	1:B:381:TRP:CD2	2.42	0.53
1:C:99:ILE:HG13	1:B:136:ASP:HA	1.90	0.53
1:E:102:ARG:NH1	1:E:143:GLN:O	2.42	0.53
1:A:378:THR:HG21	1:A:389:GLN:HE21	1.72	0.53
1:C:349:ILE:HD12	1:C:416:ILE:HG13	1.90	0.53
1:G:182:MET:HE2	1:G:183:TYR:C	2.29	0.53
1:A:330:TYR:HD1	1:A:351:VAL:HG12	1.74	0.52
1:D:367:GLN:HB2	1:D:400:ILE:HB	1.91	0.52
1:D:61:GLU:O	1:D:65:ASN:ND2	2.34	0.52
1:C:48:ILE:HD13	1:C:55:ILE:HG13	1.91	0.52
1:A:349:ILE:HD12	1:A:416:ILE:HG13	1.91	0.52
1:D:444:SER:HA	1:D:447:MET:HE2	1.91	0.52
1:H:261:PHE:HZ	1:H:290:ILE:HG23	1.74	0.52
1:D:38:LEU:HD13	1:D:59:LEU:HD11	1.92	0.52
1:D:155:TYR:OH	1:D:348:GLU:OE2	2.18	0.51
1:A:253:LEU:HG	1:B:365:LEU:HD11	1.91	0.51
1:C:38:LEU:HD13	1:C:59:LEU:HD11	1.91	0.51
1:H:349:ILE:HD12	1:H:416:ILE:HG13	1.92	0.51
1:G:235:ASP:OD1	1:G:237:THR:OG1	2.18	0.51
1:B:349:ILE:HB	1:B:414:ILE:HG13	1.91	0.51
1:G:154:THR:HB	1:G:182:MET:HG3	1.91	0.51
1:D:441:ARG:NH2	3:D:605:HOH:O	2.37	0.51
1:E:312:ILE:HD12	1:E:338:THR:HB	1.93	0.51
1:E:411:ASN:ND2	3:E:605:HOH:O	2.42	0.51
1:D:375:SER:OG	1:D:411:ASN:O	2.27	0.51
1:H:345:LYS:HB2	1:H:418:ARG:HB2	1.92	0.50
1:D:422:LYS:HB3	1:C:217:ILE:HD13	1.93	0.50
1:C:81:CYS:SG	1:C:401:LYS:HE3	2.52	0.50
1:G:349:ILE:HD12	1:G:416:ILE:HG13	1.94	0.50
1:C:298:SER:O	1:C:302:MET:HG3	2.12	0.50
1:F:121:PHE:HD1	1:F:123:PRO:HD3	1.77	0.50
1:G:27:ILE:O	1:G:29:ARG:NH2	2.44	0.50
1:G:367:GLN:HB2	1:G:400:ILE:HB	1.93	0.50
1:F:150:MET:HG2	1:F:208:THR:HB	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:ILE:HG12	1:G:188:THR:HB	1.94	0.49
1:D:379:ILE:HD11	1:D:392:LEU:HD22	1.94	0.49
1:H:367:GLN:HB2	1:H:400:ILE:HB	1.94	0.49
1:A:200:GLN:NE2	3:A:614:HOH:O	2.46	0.49
1:G:38:LEU:HD13	1:G:59:LEU:HD11	1.95	0.49
1:A:121:PHE:HB3	1:A:123:PRO:HD3	1.95	0.49
1:D:298:SER:O	1:D:302:MET:HG3	2.13	0.49
1:D:440:GLN:HG3	1:C:230:SER:HB3	1.95	0.49
1:E:85:ILE:HD12	1:E:381:TRP:CD2	2.48	0.49
1:F:367:GLN:HB2	1:F:400:ILE:HB	1.95	0.49
1:A:222:SER:HA	1:B:443:ILE:HG23	1.94	0.49
1:F:121:PHE:CD2	1:F:419:ILE:HD11	2.47	0.49
1:A:249:TYR:O	1:A:253:LEU:HD13	2.13	0.48
1:A:27:ILE:O	1:A:29:ARG:NH1	2.46	0.48
1:D:124:GLU:HB2	1:D:206:ALA:HB3	1.94	0.48
1:F:247:LEU:HG	1:F:276:PHE:HE1	1.77	0.48
1:C:414:ILE:HD12	1:C:416:ILE:HD11	1.95	0.48
1:D:349:ILE:HD12	1:D:416:ILE:HG13	1.95	0.48
1:E:113:THR:HG22	1:E:125:TRP:CD1	2.49	0.48
1:H:27:ILE:O	1:H:29:ARG:NH1	2.47	0.48
1:E:151:HIS:O	1:E:208:THR:HA	2.12	0.47
1:F:334:GLU:OE2	1:E:295:ASN:ND2	2.47	0.47
1:B:261:PHE:HZ	1:B:290:ILE:HG23	1.79	0.47
1:A:85:ILE:HD12	1:A:381:TRP:CD2	2.49	0.47
1:H:182:MET:HE2	1:H:183:TYR:C	2.34	0.47
1:F:99:ILE:HG13	1:H:136:ASP:HA	1.97	0.47
1:D:121:PHE:HB3	1:D:419:ILE:HD11	1.96	0.47
1:E:349:ILE:HD12	1:E:416:ILE:HG13	1.97	0.47
3:G:602:HOH:O	1:H:72:ARG:NH2	2.30	0.47
1:A:230:SER:HA	1:B:439:THR:HG21	1.97	0.46
1:C:382:ASN:HB3	1:C:405:PRO:HG2	1.97	0.46
1:C:121:PHE:CD2	1:C:419:ILE:HD11	2.50	0.46
1:F:144:TRP:CZ3	1:F:165:LYS:HG3	2.50	0.46
1:E:414:ILE:HD12	1:E:416:ILE:HD11	1.98	0.46
1:B:144:TRP:CZ3	1:B:165:LYS:HG3	2.51	0.46
1:B:414:ILE:HD12	1:B:416:ILE:HD11	1.97	0.46
1:A:145:ASN:HB2	1:B:449:TRP:O	2.16	0.46
1:B:64:VAL:HG21	1:B:71:GLU:HG2	1.97	0.46
1:D:121:PHE:HD2	1:D:419:ILE:HD11	1.81	0.46
1:A:367:GLN:HB2	1:A:400:ILE:HB	1.98	0.46
1:B:284:PHE:CE2	1:B:288:LYS:HE2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:NH1	1:C:143:GLN:O	2.49	0.46
1:A:330:TYR:CD1	1:A:351:VAL:HG12	2.51	0.45
1:H:85:ILE:HD12	1:H:381:TRP:CD2	2.52	0.45
1:A:77:VAL:HG13	1:B:219:GLN:NE2	2.31	0.45
1:D:436:ARG:HG3	1:C:230:SER:HB2	1.98	0.45
1:D:85:ILE:HD12	1:D:381:TRP:CD2	2.51	0.45
1:F:68:PRO:O	1:E:122:ARG:NH2	2.32	0.45
1:G:29:ARG:NE	1:G:37:GLU:OE1	2.41	0.45
1:E:345:LYS:NZ	3:E:603:HOH:O	2.40	0.45
1:H:121:PHE:CD1	1:H:123:PRO:HD3	2.51	0.45
1:H:97:SER:HA	1:H:110:TYR:O	2.17	0.45
1:A:149:PHE:CZ	1:A:213:LEU:HB3	2.52	0.44
1:E:120:PRO:HD2	1:E:121:PHE:CE2	2.51	0.44
1:F:155:TYR:OH	1:F:348:GLU:OE2	2.19	0.44
1:G:35:ALA:HA	1:G:40:VAL:HG12	1.98	0.44
1:D:154:THR:HB	1:D:182:MET:HG3	2.00	0.44
1:G:423:ILE:HA	1:G:427:SER:HB2	2.00	0.44
1:A:413:LYS:NZ	3:A:612:HOH:O	2.43	0.44
1:E:125:TRP:CD2	1:E:205:LEU:HD21	2.52	0.44
1:A:23:ILE:O	1:A:27:ILE:HG12	2.18	0.44
1:B:382:ASN:HB3	1:B:405:PRO:HG2	2.00	0.44
1:G:85:ILE:HD12	1:G:381:TRP:CD2	2.53	0.44
1:C:371:ASN:ND2	1:C:392:LEU:O	2.51	0.43
1:C:131:LYS:HA	1:C:194:THR:O	2.19	0.43
1:C:331:GLU:HB3	1:C:350:ASP:HB2	2.00	0.43
1:F:382:ASN:HB3	1:F:405:PRO:HG2	1.99	0.43
1:D:217:ILE:HD12	1:C:423:ILE:HG12	2.00	0.43
1:E:207:LEU:HD21	1:E:419:ILE:HG13	2.01	0.43
1:F:351:VAL:O	1:F:411:ASN:HA	2.19	0.43
1:G:149:PHE:CZ	1:G:213:LEU:HB3	2.53	0.43
1:B:298:SER:O	1:B:302:MET:HG3	2.18	0.43
1:B:207:LEU:HB2	1:B:417:LEU:HD13	2.00	0.43
1:G:121:PHE:HD1	1:G:123:PRO:HD3	1.84	0.43
1:G:429:ARG:HD3	3:H:529:HOH:O	2.18	0.43
1:H:119:ALA:HB2	1:H:399:TYR:CZ	2.54	0.43
1:C:121:PHE:CD1	1:C:123:PRO:HD3	2.52	0.43
1:C:388:TYR:OH	3:C:601:HOH:O	2.19	0.43
1:G:152:GLN:HB3	1:G:184:ILE:HG22	2.01	0.43
1:G:27:ILE:HG13	1:G:29:ARG:HG2	2.01	0.43
1:B:322:TRP:CH2	1:B:334:GLU:HG3	2.54	0.43
1:F:68:PRO:HG2	1:E:122:ARG:HH12	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:SER:O	1:A:302:MET:HG3	2.19	0.42
1:C:367:GLN:HB2	1:C:400:ILE:HB	2.01	0.42
1:H:124:GLU:N	1:H:206:ALA:O	2.50	0.42
1:B:166:ASP:OD2	1:B:170:LYS:HB3	2.19	0.42
1:D:441:ARG:NH2	1:C:146:ASN:O	2.45	0.42
1:D:223:SER:O	1:C:401:LYS:NZ	2.34	0.42
1:F:122:ARG:HB2	1:F:208:THR:OG1	2.19	0.42
1:A:67:TRP:O	1:B:117:LYS:NZ	2.53	0.42
1:B:357:LEU:HA	1:B:357:LEU:HD12	1.83	0.42
1:C:121:PHE:HB3	1:C:419:ILE:HD11	2.00	0.42
1:D:100:MET:HB2	1:D:108:TYR:HB2	2.01	0.42
1:E:154:THR:HG23	1:E:204:ILE:HB	2.02	0.42
1:G:324:TYR:HA	1:G:325:PRO:HA	1.88	0.42
1:C:379:ILE:HD12	1:C:408:PHE:CE1	2.55	0.42
1:G:433:PHE:O	1:H:310:LYS:HE2	2.20	0.42
1:D:227:ASP:OD1	1:D:227:ASP:N	2.46	0.42
1:E:284:PHE:CE2	1:E:288:LYS:HE3	2.55	0.42
1:H:131:LYS:HA	1:H:194:THR:O	2.20	0.42
1:E:27:ILE:O	1:E:29:ARG:NH1	2.52	0.42
1:E:349:ILE:HB	1:E:414:ILE:HG13	2.01	0.42
1:E:125:TRP:HE3	1:E:203:LEU:HD11	1.85	0.41
1:E:125:TRP:CE2	1:E:205:LEU:HD21	2.55	0.41
1:A:144:TRP:CH2	1:A:163:TYR:HB3	2.55	0.41
1:E:28:LYS:HD2	1:E:28:LYS:N	2.35	0.41
1:G:182:MET:CE	1:G:184:ILE:HB	2.45	0.41
1:H:121:PHE:HD1	1:H:123:PRO:HD3	1.84	0.41
1:G:423:ILE:HD13	1:H:221:LEU:HD13	2.02	0.41
1:H:227:ASP:O	1:H:231:GLN:HG3	2.19	0.41
1:A:184:ILE:HD11	1:A:188:THR:HB	2.02	0.41
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.81	0.41
1:G:66:ILE:HG13	1:G:67:TRP:CD1	2.55	0.41
1:H:353:SER:O	1:H:410:GLY:N	2.39	0.41
1:C:21:LEU:HD13	1:C:49:ILE:HD13	2.02	0.41
1:A:149:PHE:HZ	1:A:213:LEU:HB3	1.86	0.41
1:F:362:LYS:HD2	3:E:601:HOH:O	2.19	0.41
1:B:109:GLU:HB3	1:B:127:LEU:HB3	2.03	0.41
1:E:379:ILE:HD11	1:E:392:LEU:HD22	2.02	0.41
1:H:347:PHE:HB2	1:H:416:ILE:HB	2.01	0.41
1:H:144:TRP:CZ3	1:H:165:LYS:HG3	2.56	0.41
1:B:213:LEU:O	1:B:218:GLN:HB2	2.20	0.41
1:F:314:LYS:NZ	3:F:513:HOH:O	2.43	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:GLU:HB2	1:H:206:ALA:HB3	2.01	0.41
1:G:369:VAL:HB	1:G:398:ALA:HB3	2.03	0.41
1:B:322:TRP:HH2	1:B:334:GLU:HG3	1.86	0.40
1:G:331:GLU:HB3	1:G:350:ASP:HB2	2.03	0.40
1:G:422:LYS:HE2	1:H:216:ASP:OD2	2.21	0.40
1:B:234:LEU:HB3	1:B:245:SER:HB3	2.04	0.40
1:C:159:GLU:HB3	1:C:195:ARG:CZ	2.51	0.40
1:F:356:ASP:HB3	1:F:409:ARG:NE	2.28	0.40
1:F:367:GLN:OE1	1:F:418:ARG:NE	2.49	0.40
1:H:154:THR:HB	1:H:182:MET:HG3	2.02	0.40
1:A:55:ILE:HG12	1:A:56:SER:H	1.87	0.40
1:C:375:SER:OG	1:C:411:ASN:O	2.28	0.40
1:D:150:MET:HG2	1:D:208:THR:HB	2.03	0.40
1:A:117:LYS:NZ	1:B:69:VAL:O	2.51	0.40
1:D:98:ARG:NH1	1:D:112:ASP:OD1	2.51	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)
3:A:727:HOH:O	3:D:733:HOH:O 4_546	2.15	0.05

## 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	440/457 (96%)	432 (98%)	8 (2%)	0	100	100
1	B	439/457 (96%)	430 (98%)	9 (2%)	0	100	100
1	C	437/457 (96%)	430 (98%)	7 (2%)	0	100	100
1	D	440/457 (96%)	432 (98%)	8 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	439/457 (96%)	433 (99%)	6 (1%)	0	100	100
1	F	393/457 (86%)	381 (97%)	9 (2%)	3 (1%)	22	31
1	G	440/457 (96%)	433 (98%)	7 (2%)	0	100	100
1	H	427/457 (93%)	416 (97%)	11 (3%)	0	100	100
All	All	3455/3656 (94%)	3387 (98%)	65 (2%)	3 (0%)	55	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	355	GLU
1	F	421	GLY
1	F	422	LYS

### 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	375/409 (92%)	370 (99%)	5 (1%)	73	86
1	B	370/409 (90%)	366 (99%)	4 (1%)	78	89
1	C	358/409 (88%)	354 (99%)	4 (1%)	78	89
1	D	364/409 (89%)	362 (100%)	2 (0%)	91	96
1	E	354/409 (87%)	351 (99%)	3 (1%)	85	93
1	F	320/409 (78%)	316 (99%)	4 (1%)	73	86
1	G	366/409 (90%)	362 (99%)	4 (1%)	78	89
1	H	352/409 (86%)	349 (99%)	3 (1%)	82	91
All	All	2859/3272 (87%)	2830 (99%)	29 (1%)	80	90

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	182	MET
1	A	217	ILE
1	A	237	THR
1	A	255	ASN
1	D	182	MET
1	D	255	ASN
1	C	182	MET
1	C	237	THR
1	C	255	ASN
1	C	351	VAL
1	F	182	MET
1	F	237	THR
1	F	255	ASN
1	F	351	VAL
1	G	40	VAL
1	G	237	THR
1	G	255	ASN
1	G	351	VAL
1	B	41	SER
1	B	182	MET
1	B	255	ASN
1	B	446	THR
1	E	182	MET
1	E	217	ILE
1	E	255	ASN
1	H	184	ILE
1	H	255	ASN
1	H	351	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	GLN
1	D	266	ASN
1	D	389	GLN
1	F	329	ASN
1	G	389	GLN
1	B	219	GLN
1	B	389	GLN
1	H	53	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	442/457 (96%)	-0.10	12 (2%) 55 56	29, 43, 68, 78	0
1	B	441/457 (96%)	-0.10	11 (2%) 58 59	37, 47, 60, 70	0
1	C	439/457 (96%)	0.12	26 (5%) 23 25	33, 45, 93, 102	0
1	D	441/457 (96%)	-0.03	17 (3%) 40 43	29, 40, 74, 91	0
1	E	441/457 (96%)	0.29	31 (7%) 17 18	32, 50, 76, 86	0
1	F	397/457 (86%)	0.33	28 (7%) 17 17	33, 52, 75, 85	0
1	G	442/457 (96%)	0.02	8 (1%) 69 70	31, 48, 65, 71	0
1	H	429/457 (93%)	0.13	12 (2%) 53 55	41, 53, 64, 71	0
All	All	3472/3656 (94%)	0.08	145 (4%) 37 39	29, 48, 73, 102	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	448	GLN	7.3
1	D	25	ASN	5.6
1	C	10	ASP	5.5
1	F	435	GLY	5.5
1	F	58	SER	5.1
1	C	11	SER	4.9
1	D	42	ILE	4.8
1	E	47	SER	4.8
1	E	451	ASP	4.7
1	G	274	ASP	4.5
1	C	42	ILE	4.5
1	E	42	ILE	4.4
1	C	40	VAL	4.4
1	C	66	ILE	4.4
1	F	24	LEU	4.3
1	C	36	ASN	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	4.2
1	C	41	SER	4.1
1	D	41	SER	4.1
1	E	11	SER	4.1
1	H	436	ARG	4.0
1	D	36	ASN	3.7
1	H	266	ASN	3.7
1	G	285	ASP	3.7
1	F	355	GLU	3.6
1	F	436	ARG	3.6
1	F	57	PRO	3.6
1	D	65	ASN	3.5
1	E	266	ASN	3.5
1	F	266	ASN	3.5
1	H	435	GLY	3.5
1	F	434	VAL	3.5
1	A	43	GLU	3.5
1	F	78	SER	3.4
1	D	32	GLU	3.4
1	D	451	ASP	3.4
1	B	266	ASN	3.4
1	E	280	LYS	3.4
1	B	11	SER	3.3
1	H	45	ILE	3.3
1	A	355	GLU	3.3
1	A	266	ASN	3.3
1	B	50	SER	3.3
1	F	352	SER	3.3
1	F	25	ASN	3.2
1	E	239	HIS	3.2
1	C	24	LEU	3.2
1	E	274	ASP	3.2
1	F	287	LEU	3.2
1	D	43	GLU	3.1
1	E	450	PHE	3.1
1	E	41	SER	3.0
1	F	63	ALA	3.0
1	C	25	ASN	3.0
1	E	352	SER	2.9
1	C	35	ALA	2.9
1	E	281	LEU	2.9
1	E	36	ASN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	242	ALA	2.9
1	E	226	LEU	2.9
1	E	40	VAL	2.8
1	D	39	GLY	2.8
1	H	41	SER	2.8
1	C	68	PRO	2.8
1	F	439	THR	2.8
1	C	39	GLY	2.8
1	C	63	ALA	2.7
1	F	391	SER	2.7
1	H	11	SER	2.7
1	C	30	ARG	2.7
1	E	56	SER	2.7
1	D	33	ASP	2.7
1	F	21	LEU	2.7
1	F	384	GLU	2.7
1	E	167	PRO	2.7
1	D	285	ASP	2.7
1	E	187	PHE	2.7
1	D	24	LEU	2.6
1	C	12	TYR	2.6
1	B	274	ASP	2.6
1	E	58	SER	2.6
1	D	23	ILE	2.5
1	C	15	ARG	2.5
1	A	285	ASP	2.5
1	F	168	GLU	2.5
1	H	200	GLN	2.5
1	A	10	ASP	2.5
1	C	58	SER	2.5
1	H	374	ASP	2.5
1	E	26	ASP	2.5
1	F	374	ASP	2.4
1	F	59	LEU	2.4
1	C	285	ASP	2.4
1	F	281	LEU	2.4
1	E	242	ALA	2.4
1	H	277	THR	2.4
1	E	66	ILE	2.4
1	E	148	HIS	2.4
1	B	277	THR	2.3
1	B	327	SER	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	279	LYS	2.3
1	C	196	ASP	2.3
1	B	47	SER	2.3
1	G	355	GLU	2.3
1	A	273	ALA	2.3
1	C	47	SER	2.3
1	E	218	GLN	2.3
1	F	274	ASP	2.3
1	F	82	SER	2.3
1	F	64	VAL	2.3
1	H	239	HIS	2.3
1	C	32	GLU	2.3
1	G	451	ASP	2.3
1	D	58	SER	2.3
1	E	38	LEU	2.3
1	E	120	PRO	2.2
1	E	65	ASN	2.2
1	E	125	TRP	2.2
1	C	23	ILE	2.2
1	G	36	ASN	2.2
1	F	68	PRO	2.2
1	E	35	ALA	2.2
1	G	30	ARG	2.2
1	A	47	SER	2.2
1	A	45	ILE	2.2
1	D	66	ILE	2.1
1	C	50	SER	2.1
1	A	32	GLU	2.1
1	B	446	THR	2.1
1	H	110	TYR	2.1
1	A	354	SER	2.1
1	A	239	HIS	2.1
1	D	374	ASP	2.1
1	D	64	VAL	2.1
1	F	217	ILE	2.1
1	G	239	HIS	2.1
1	F	275	PHE	2.1
1	B	91	GLN	2.1
1	B	440	GLN	2.1
1	C	374	ASP	2.0
1	G	43	GLU	2.0
1	E	39	GLY	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	199	SER	2.0
1	C	33	ASP	2.0
1	E	263	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	FE	C	501	1/1	0.96	0.27	4.34	72,72,72,72	0
2	FE	A	501	1/1	0.94	0.12	-0.54	63,63,63,63	0
2	FE	D	501	1/1	0.97	0.11	-0.66	54,54,54,54	1
2	FE	E	501	1/1	0.98	0.02	-2.28	55,55,55,55	0
2	FE	G	501	1/1	0.96	0.09	-	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.