



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:56 PM UTC

PDB ID : 5YXY / pdb_00005yxy
Title : Crystal structure of the HyhL-HypA complex (form I)
Authors : Kwon, S.; Watanabe, S.; Nishitani, Y.; Miki, K.
Deposited on : 2017-12-07
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

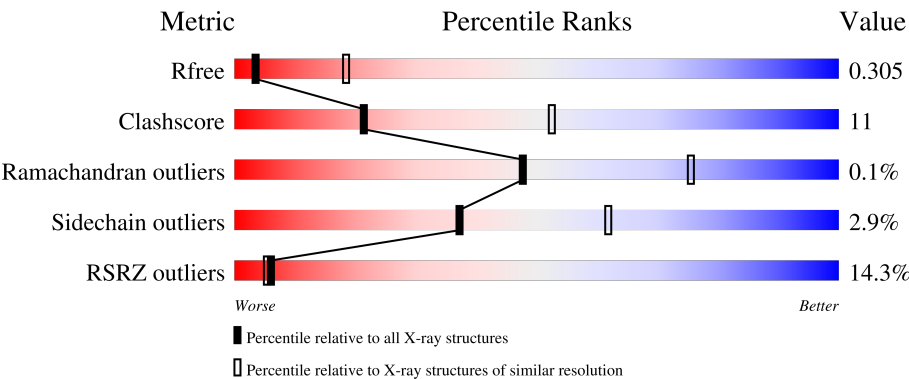
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	12% 74% 19% • 6%
1	B	428	22% 74% 17% • 8%
1	C	428	12% 71% 22% • 5%
2	D	139	5% 78% 10% • 11%
2	E	139	8% 73% 14% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	139	6% 77% 9% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11198 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 Cytosolic NiFe-hydrogenase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			2851	1814	476	545	16			
1	B	394	Total	C	N	O	S	0	0	0
			2697	1718	454	510	15			
1	C	406	Total	C	N	O	S	0	0	0
			2940	1887	492	546	15			

- Molecule 2 is a protein called Probable hydrogenase nickel incorporation protein HypA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	124	Total	C	N	O	S	0	0	0
			917	587	155	170	5			
2	E	123	Total	C	N	O	S	0	0	0
			925	594	153	173	5			
2	F	121	Total	C	N	O	S	0	0	0
			865	555	139	166	5			

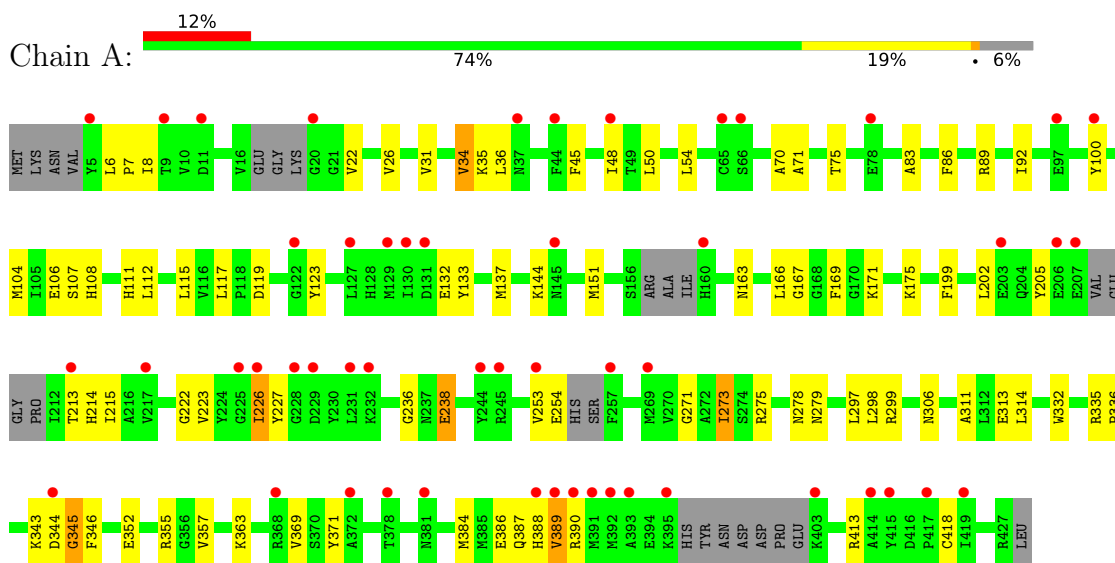
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

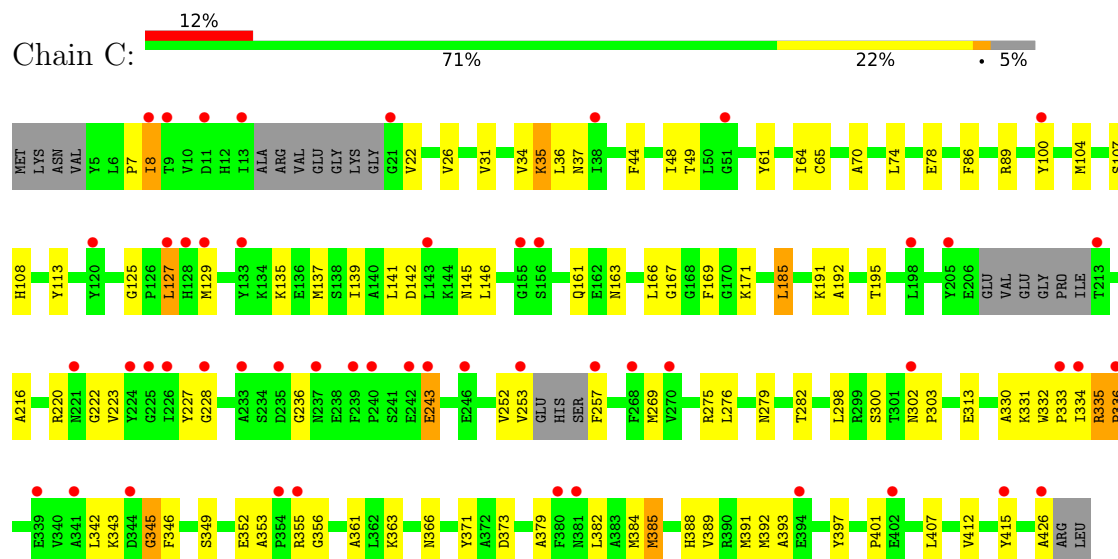
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

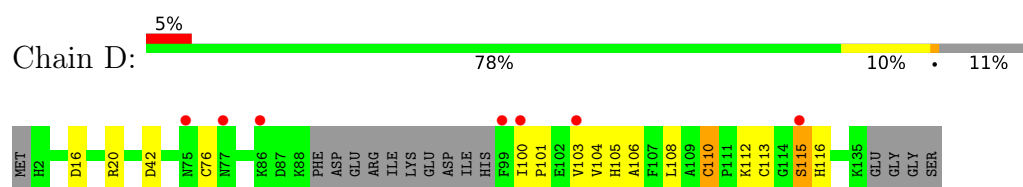
- Molecule 1: Cytosolic NiFe-hydrogenase, alpha subunit



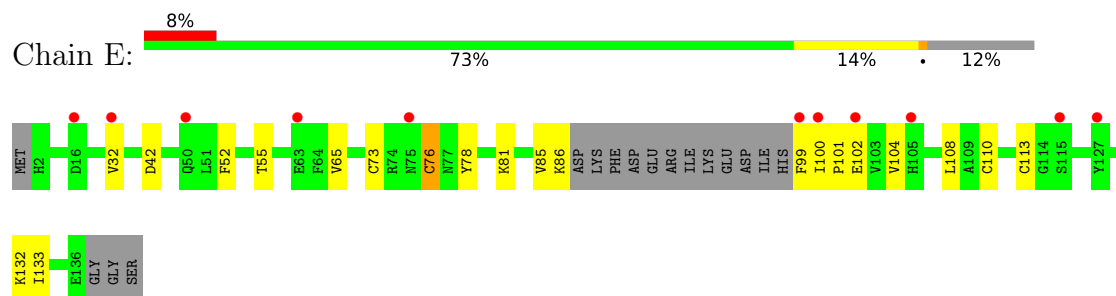
- Molecule 1: Cytosolic NiFe-hydrogenase, alpha subunit



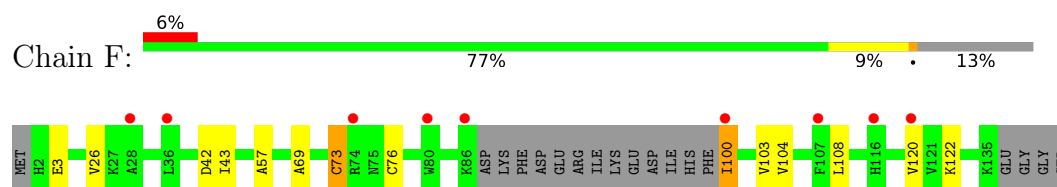
- Molecule 2: Probable hydrogenase nickel incorporation protein HypA



- Molecule 2: Probable hydrogenase nickel incorporation protein HypA



- Molecule 2: Probable hydrogenase nickel incorporation protein HypA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	245.31 Å 261.43 Å 134.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 3.30 48.22 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.22-3.30) 98.9 (48.22-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.33 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.305 , 0.321 (Not available) , 0.305	Depositor DCC
R_{free} test set	3185 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11198	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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:
ZN

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	0.39	0/2898	0.83	2/3953 (0.1%)
1	B	0.37	0/2741	0.86	4/3743 (0.1%)
1	C	0.44	3/2996 (0.1%)	0.89	8/4079 (0.2%)
2	D	0.37	0/933	0.81	1/1267 (0.1%)
2	E	0.32	0/941	0.75	0/1276
2	F	0.32	0/881	0.78	2/1203 (0.2%)
All	All	0.39	3/11390 (0.0%)	0.84	17/15521 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	401	PRO	N-CD	-7.12	1.37	1.47
1	C	335	ARG	C-N	5.77	1.41	1.33
1	C	336	PRO	N-CD	5.26	1.55	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	ALA	N-CA-C	-8.60	98.37	110.50
1	B	332	TRP	CA-C-N	-8.51	109.20	119.84
1	B	332	TRP	C-N-CA	-8.51	109.20	119.84
1	C	345	GLY	N-CA-C	6.89	121.59	112.77
2	F	100	ILE	CA-C-N	-6.89	111.34	118.85
2	F	100	ILE	C-N-CA	-6.89	111.34	118.85
1	C	243	GLU	N-CA-C	6.34	119.99	111.24
1	A	387	GLN	N-CA-C	6.26	118.19	111.36
2	D	115	SER	N-CA-C	6.25	121.12	111.56
1	B	393	ALA	N-CA-C	-6.20	106.03	113.97
1	A	345	GLY	N-CA-C	-6.17	104.15	111.36
1	C	335	ARG	CA-C-N	-6.12	113.67	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	ARG	C-N-CA	-6.12	113.67	119.85
1	C	331	LYS	N-CA-C	6.02	119.86	111.74
1	C	125	GLY	CA-C-N	5.31	125.07	119.76
1	C	125	GLY	C-N-CA	5.31	125.07	119.76
1	B	392	MET	N-CA-C	-5.11	106.63	112.92

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	2851	0	2573	58	0
1	B	2697	0	2341	57	0
1	C	2940	0	2746	70	0
2	D	917	0	850	19	0
2	E	925	0	870	24	0
2	F	865	0	760	9	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	11198	0	10140	232	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 11.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:CYS:HB3	2:E:113:CYS:SG	1.57	1.43
2:E:76:CYS:CB	2:E:113:CYS:SG	2.27	1.21
1:A:123:TYR:CE2	1:A:132:GLU:OE1	1.92	1.21
1:A:384:MET:HE3	1:A:388:HIS:NE2	1.56	1.20
1:B:26:VAL:O	1:B:426:ALA:CB	2.03	1.07
1:A:238:GLU:OE1	1:A:238:GLU:N	1.88	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:76:CYS:SG	2:E:78:TYR:HB3	1.95	1.05
2:E:76:CYS:SG	2:E:78:TYR:CB	2.44	1.04
1:A:123:TYR:HE2	1:A:132:GLU:OE1	1.40	0.98
1:B:26:VAL:O	1:B:426:ALA:HB1	1.64	0.98
1:C:332:TRP:CD2	1:C:333:PRO:HA	2.05	0.91
1:A:236:GLY:O	1:A:278:ASN:ND2	2.04	0.91
2:E:76:CYS:SG	2:E:78:TYR:HB2	2.12	0.90
1:A:346:PHE:HD1	1:A:363:LYS:HB2	1.38	0.89
2:E:85:VAL:O	2:E:86:LYS:HG2	1.74	0.88
1:A:384:MET:CE	1:A:388:HIS:NE2	2.36	0.88
2:D:104:VAL:CG1	2:D:108:LEU:HB2	2.05	0.86
2:D:76:CYS:HB3	2:D:113:CYS:SG	2.21	0.81
2:E:99:PHE:C	2:E:101:PRO:HD3	2.07	0.80
1:C:269:MET:HB2	1:C:384:MET:HG2	1.64	0.79
1:A:106:GLU:HG3	1:A:144:LYS:HD2	1.69	0.75
1:B:363:LYS:HB3	1:B:371:TYR:HB3	1.69	0.75
1:B:203:GLU:HG2	1:B:205:TYR:H	1.52	0.75
1:A:169:PHE:H	1:A:336:PRO:HB3	1.51	0.74
1:A:205:TYR:O	1:A:213:THR:HA	1.87	0.74
1:B:246:GLU:HG2	1:B:247:HIS:H	1.52	0.74
1:C:363:LYS:HB3	1:C:371:TYR:HB3	1.70	0.73
2:E:76:CYS:HB2	2:E:113:CYS:SG	2.29	0.72
1:B:169:PHE:H	1:B:336:PRO:HB3	1.53	0.72
1:A:363:LYS:HB3	1:A:371:TYR:HB3	1.71	0.71
1:A:346:PHE:CD1	1:A:363:LYS:HB2	2.25	0.71
2:E:76:CYS:HG	2:E:78:TYR:HB3	1.54	0.71
2:D:104:VAL:HG12	2:D:108:LEU:HB2	1.72	0.71
2:E:104:VAL:HG13	2:E:108:LEU:HB2	1.73	0.70
1:B:5:TYR:HA	2:E:132:LYS:HD3	1.74	0.69
1:A:107:SER:OG	1:A:355:ARG:NH1	2.25	0.69
1:C:393:ALA:O	1:C:397:TYR:N	2.26	0.69
2:E:100:ILE:N	2:E:101:PRO:HD3	2.08	0.68
1:C:275:ARG:HD3	1:C:352:GLU:HG2	1.74	0.68
2:D:115:SER:O	2:D:116:HIS:HB2	1.91	0.68
1:A:26:VAL:HG12	1:A:31:VAL:HG12	1.76	0.67
1:C:332:TRP:CG	1:C:333:PRO:HA	2.28	0.67
1:B:246:GLU:HG2	1:B:247:HIS:N	2.10	0.67
2:D:104:VAL:CG1	2:D:108:LEU:HD22	2.25	0.67
1:A:215:ILE:HD12	1:A:299:ARG:HE	1.59	0.67
1:C:141:LEU:O	1:C:145:ASN:ND2	2.27	0.67
1:C:142:ASP:OD2	1:C:191:LYS:NZ	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TYR:CZ	1:A:132:GLU:OE1	2.48	0.67
1:A:343:LYS:HG2	1:A:344:ASP:N	2.10	0.66
2:D:104:VAL:HG13	2:D:108:LEU:HD22	1.78	0.65
2:E:85:VAL:O	2:E:86:LYS:CG	2.44	0.65
1:C:127:LEU:HD23	1:C:129:MET:H	1.61	0.65
2:E:100:ILE:N	2:E:101:PRO:CD	2.60	0.65
1:B:215:ILE:HD11	1:B:301:THR:OG1	1.97	0.64
1:C:333:PRO:O	1:C:334:ILE:HG22	1.97	0.64
2:D:104:VAL:HG13	2:D:108:LEU:HB2	1.80	0.64
1:C:220:ARG:NH1	1:C:300:SER:O	2.30	0.64
1:C:223:VAL:O	1:C:279:ASN:ND2	2.31	0.63
1:B:276:LEU:HD21	1:B:298:LEU:HD13	1.80	0.62
1:B:363:LYS:HG2	1:B:370:SER:HB3	1.81	0.62
1:B:100:TYR:OH	1:B:352:GLU:O	2.12	0.62
1:A:100:TYR:OH	1:A:352:GLU:O	2.07	0.62
1:A:89:ARG:NH2	1:A:335:ARG:O	2.33	0.62
1:A:132:GLU:HG2	1:A:133:TYR:HB2	1.82	0.61
1:C:334:ILE:O	1:C:334:ILE:HG23	2.00	0.61
1:B:119:ASP:HB3	1:B:410:MET:HE2	1.83	0.60
2:D:103:VAL:HG12	2:D:103:VAL:O	2.01	0.60
1:B:22:VAL:HG13	1:B:36:LEU:HB3	1.82	0.60
1:C:86:PHE:CE2	1:C:167:GLY:HA2	2.37	0.60
2:E:85:VAL:C	2:E:86:LYS:HG2	2.26	0.60
2:F:73:CYS:SG	2:F:76:CYS:HB2	2.41	0.59
1:B:89:ARG:NH2	1:B:335:ARG:O	2.34	0.59
1:A:275:ARG:NH1	1:A:313:GLU:OE1	2.37	0.58
1:A:386:GLU:O	1:A:389:VAL:HG22	2.03	0.58
1:C:26:VAL:O	1:C:426:ALA:HA	2.04	0.58
1:C:345:GLY:O	1:C:363:LYS:HA	2.04	0.58
2:E:76:CYS:CA	2:E:113:CYS:SG	2.92	0.57
1:B:133:TYR:CE2	1:B:137:MET:HG2	2.40	0.57
1:C:107:SER:OG	1:C:355:ARG:NH1	2.37	0.57
1:A:89:ARG:H	1:A:92:ILE:HD11	1.70	0.57
1:C:161:GLN:OE1	1:C:161:GLN:N	2.38	0.57
1:A:273:ILE:HG12	1:A:306:ASN:HA	1.86	0.56
1:B:45:PHE:HA	1:B:48:ILE:HG12	1.87	0.56
1:C:192:ALA:O	1:C:195:THR:OG1	2.16	0.56
1:A:45:PHE:HA	1:A:48:ILE:HG12	1.88	0.56
1:C:104:MET:SD	1:C:108:HIS:NE2	2.79	0.55
1:B:419:ILE:HG13	1:B:420:SER:N	2.21	0.55
1:C:361:ALA:HB3	1:C:373:ASP:HB3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ARG:HA	1:B:393:ALA:HB3	1.88	0.55
2:E:104:VAL:HG22	2:E:108:LEU:HD22	1.88	0.55
1:B:343:LYS:HG2	1:B:366:ASN:H	1.71	0.55
1:A:54:LEU:HD22	1:A:166:LEU:HD22	1.88	0.54
1:C:44:PHE:CZ	1:C:48:ILE:HD11	2.42	0.54
1:C:222:GLY:O	1:C:236:GLY:N	2.33	0.54
1:C:275:ARG:HH21	1:C:352:GLU:HG3	1.71	0.54
1:B:26:VAL:O	1:B:426:ALA:HB3	2.01	0.54
1:A:223:VAL:O	1:A:279:ASN:ND2	2.40	0.54
1:C:146:LEU:HD21	1:C:185:LEU:HD12	1.91	0.53
1:A:83:ALA:O	1:A:345:GLY:HA3	2.09	0.53
1:A:133:TYR:HD1	1:A:137:MET:HG3	1.73	0.53
1:C:100:TYR:OH	1:C:352:GLU:O	2.05	0.53
1:B:215:ILE:HG13	1:B:301:THR:HB	1.91	0.53
1:B:185:LEU:HD22	1:B:322:ILE:HB	1.90	0.52
1:C:343:LYS:HG3	1:C:366:ASN:H	1.72	0.52
1:A:133:TYR:CD1	1:A:137:MET:HG3	2.45	0.52
2:E:101:PRO:O	2:E:102:GLU:HB2	2.08	0.52
1:C:22:VAL:HG13	1:C:36:LEU:HB3	1.91	0.52
1:A:175:LYS:NZ	1:A:332:TRP:O	2.41	0.52
1:C:169:PHE:H	1:C:336:PRO:HB3	1.75	0.51
1:C:37:ASN:OD1	1:C:37:ASN:N	2.43	0.51
2:F:3:GLU:HG2	2:F:43:ILE:HB	1.90	0.51
1:B:396:HIS:O	1:B:396:HIS:ND1	2.42	0.51
1:C:61:TYR:O	1:C:64:ILE:HD12	2.10	0.51
1:C:379:ALA:O	1:C:382:LEU:HG	2.10	0.51
1:A:214:HIS:O	1:A:390:ARG:NH2	2.43	0.51
2:D:16:ASP:OD2	2:D:20:ARG:NH2	2.44	0.50
1:B:215:ILE:HG13	1:B:301:THR:O	2.11	0.50
1:C:139:ILE:HD12	1:C:191:LYS:HB3	1.94	0.50
1:C:385:MET:HE3	1:C:412:VAL:HG22	1.94	0.50
1:C:276:LEU:HD13	1:C:298:LEU:HD13	1.94	0.50
1:A:35:LYS:HD3	1:A:253:VAL:HA	1.94	0.50
1:B:214:HIS:O	1:B:215:ILE:C	2.55	0.49
1:C:353:ALA:N	1:C:356:GLY:O	2.35	0.49
1:B:215:ILE:HG13	1:B:301:THR:CB	2.41	0.49
2:D:100:ILE:N	2:D:101:PRO:CD	2.76	0.49
1:B:343:LYS:HE3	1:B:365:GLU:HG3	1.94	0.49
1:C:78:GLU:CD	1:C:349:SER:HG	2.20	0.49
1:B:353:ALA:N	1:B:356:GLY:O	2.39	0.49
2:E:76:CYS:N	2:E:113:CYS:SG	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:SD	1:A:108:HIS:NE2	2.86	0.48
1:C:127:LEU:HD13	1:C:137:MET:HE2	1.94	0.48
1:C:70:ALA:HB2	1:C:161:GLN:NE2	2.27	0.48
1:C:191:LYS:O	1:C:195:THR:HG23	2.13	0.48
1:B:261:SER:OG	1:B:380:PHE:HA	2.14	0.48
1:B:120:TYR:CZ	1:B:202:LEU:HD21	2.49	0.48
1:C:44:PHE:CE2	2:F:43:ILE:HG12	2.48	0.48
2:D:104:VAL:O	2:D:106:ALA:N	2.47	0.48
1:A:311:ALA:O	1:A:314:LEU:HB2	2.14	0.48
1:B:215:ILE:CD1	1:B:301:THR:OG1	2.61	0.47
1:C:343:LYS:O	1:C:345:GLY:N	2.47	0.47
1:B:116:VAL:HG21	1:B:199:PHE:CZ	2.49	0.47
1:A:71:ALA:O	1:A:75:THR:HG22	2.14	0.47
1:C:216:ALA:HB2	1:C:391:MET:HE1	1.97	0.47
2:D:76:CYS:CB	2:D:113:CYS:SG	2.95	0.47
2:D:104:VAL:HG13	2:D:108:LEU:HD13	1.96	0.47
2:F:26:VAL:HG12	2:F:57:ALA:HA	1.95	0.47
2:D:104:VAL:HG11	2:D:108:LEU:HD22	1.95	0.47
1:A:271:GLY:O	1:A:275:ARG:HD3	2.16	0.46
1:C:113:TYR:OH	1:C:195:THR:HG22	2.14	0.46
1:A:215:ILE:HD12	1:A:299:ARG:NE	2.29	0.46
1:B:47:ALA:HB1	1:C:7:PRO:HG2	1.96	0.46
1:B:24:ILE:HG12	1:B:34:VAL:HG23	1.97	0.46
1:C:227:TYR:O	1:C:228:GLY:C	2.57	0.46
2:D:42:ASP:OD1	2:D:42:ASP:N	2.49	0.46
2:E:52:PHE:O	2:E:55:THR:HG22	2.16	0.46
1:B:50:LEU:HD23	1:C:8:ILE:HA	1.98	0.45
1:B:385:MET:O	1:B:389:VAL:HG23	2.17	0.45
1:C:385:MET:O	1:C:389:VAL:HG23	2.16	0.45
1:A:369:VAL:O	1:B:9:THR:HG21	2.16	0.45
1:C:49:THR:HG21	1:C:61:TYR:CE1	2.52	0.45
1:A:89:ARG:HH22	1:A:335:ARG:H	1.64	0.45
1:C:166:LEU:HD12	1:C:166:LEU:H	1.82	0.45
2:E:73:CYS:HB2	2:E:110:CYS:HB2	1.99	0.45
1:B:120:TYR:CE2	1:B:202:LEU:HD21	2.52	0.44
1:B:133:TYR:CD2	1:B:133:TYR:O	2.70	0.44
2:D:104:VAL:CG1	2:D:108:LEU:CB	2.89	0.44
2:D:110:CYS:SG	2:D:112:LYS:N	2.85	0.44
1:C:135:LYS:O	1:C:139:ILE:HG12	2.17	0.44
1:B:283:LEU:HD11	1:B:312:LEU:HD21	1.99	0.44
1:B:283:LEU:HD23	1:B:284:TYR:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HD22	1:C:385:MET:HE2	1.98	0.44
1:C:89:ARG:NH2	1:C:335:ARG:O	2.48	0.44
1:C:253:VAL:HB	1:C:257:PHE:CE1	2.53	0.44
1:B:302:ASN:HA	1:B:303:PRO:HD3	1.79	0.44
1:A:163:ASN:ND2	1:A:171:LYS:O	2.29	0.44
1:A:384:MET:HE3	1:A:388:HIS:CD2	2.43	0.44
1:C:388:HIS:ND1	1:C:415:TYR:OH	2.32	0.43
1:B:133:TYR:HE2	1:B:137:MET:HG2	1.81	0.43
2:F:100:ILE:HG22	2:F:100:ILE:O	2.18	0.43
1:A:119:ASP:OD2	1:A:413:ARG:NH1	2.51	0.43
1:A:226:ILE:CG1	1:A:227:TYR:N	2.81	0.43
1:C:392:MET:HE3	1:C:407:LEU:HD13	2.00	0.43
1:A:386:GLU:O	1:A:389:VAL:CG2	2.66	0.43
2:E:100:ILE:HG22	2:E:100:ILE:O	2.17	0.43
1:C:26:VAL:HA	1:C:31:VAL:HA	1.99	0.43
1:C:31:VAL:HG11	1:C:393:ALA:HB1	2.00	0.43
2:F:42:ASP:OD1	2:F:42:ASP:N	2.50	0.43
1:B:343:LYS:HE2	1:B:343:LYS:HB3	1.83	0.43
1:C:74:LEU:HD13	1:C:100:TYR:HB2	2.00	0.42
2:F:100:ILE:HA	2:F:103:VAL:HB	2.01	0.42
1:A:335:ARG:HA	1:A:336:PRO:HD3	1.80	0.42
1:B:243:GLU:O	1:B:243:GLU:HG2	2.18	0.42
1:C:303:PRO:HG3	1:C:388:HIS:CE1	2.54	0.42
1:A:273:ILE:HD13	1:A:273:ILE:HA	1.87	0.42
1:B:378:THR:O	1:B:382:LEU:HG	2.19	0.42
2:D:104:VAL:HG13	2:D:108:LEU:CD2	2.49	0.42
1:C:382:LEU:O	1:C:385:MET:HG2	2.20	0.42
2:D:104:VAL:O	2:D:105:HIS:C	2.62	0.42
1:A:86:PHE:CE2	1:A:167:GLY:HA2	2.55	0.42
1:A:34:VAL:HG21	1:A:389:VAL:HG21	2.02	0.42
1:C:279:ASN:O	1:C:282:THR:OG1	2.31	0.42
1:B:243:GLU:OE1	1:B:243:GLU:N	2.53	0.42
1:B:361:ALA:HB3	1:B:373:ASP:HB3	2.02	0.42
1:C:346:PHE:HD1	1:C:363:LYS:HB2	1.84	0.42
1:B:112:LEU:HD13	1:B:199:PHE:CE1	2.55	0.42
1:A:199:PHE:CD2	1:A:202:LEU:HD21	2.55	0.41
1:B:118:PRO:HG3	1:B:127:LEU:HD11	2.02	0.41
2:E:32:VAL:HG22	2:E:65:VAL:HB	2.01	0.41
1:B:203:GLU:HG2	1:B:205:TYR:N	2.28	0.41
1:C:302:ASN:HA	1:C:303:PRO:HD3	1.82	0.41
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LEU:O	1:B:116:VAL:HG22	2.20	0.41
1:B:387:GLN:O	1:B:391:MET:HG3	2.20	0.41
1:B:400:ASP:HB2	1:B:404:LEU:CD2	2.51	0.41
2:F:104:VAL:O	2:F:108:LEU:HB2	2.21	0.41
1:A:22:VAL:HG12	1:A:36:LEU:HB2	2.03	0.41
1:C:35:LYS:NZ	1:C:252:VAL:O	2.54	0.41
1:A:70:ALA:HB2	1:A:151:MET:HE3	2.01	0.41
1:A:112:LEU:HB3	1:A:199:PHE:CZ	2.56	0.41
1:C:163:ASN:OD1	1:C:171:LYS:N	2.52	0.41
1:C:392:MET:HE2	1:C:407:LEU:HB3	2.03	0.41
2:E:42:ASP:OD1	2:E:42:ASP:N	2.51	0.41
1:C:275:ARG:HE	1:C:313:GLU:CD	2.26	0.40
1:B:332:TRP:C	1:B:334:ILE:H	2.29	0.40
1:C:78:GLU:OE1	1:C:349:SER:OG	2.36	0.40
1:A:6:LEU:HA	1:A:7:PRO:HD3	1.80	0.40
1:A:111:HIS:O	1:A:115:LEU:HB2	2.22	0.40
1:A:222:GLY:O	1:A:236:GLY:N	2.54	0.40
2:F:69:ALA:HA	2:F:122:LYS:O	2.21	0.40
1:A:343:LYS:CG	1:A:344:ASP:N	2.80	0.40
1:B:40:GLU:N	1:B:40:GLU:OE1	2.55	0.40
1:C:342:LEU:HD23	1:C:342:LEU:HA	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/428 (92%)	384 (98%)	8 (2%)	0	100	100
1	B	376/428 (88%)	366 (97%)	8 (2%)	2 (0%)	24	55
1	C	398/428 (93%)	388 (98%)	10 (2%)	0	100	100
2	D	120/139 (86%)	115 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	119/139 (86%)	118 (99%)	1 (1%)	0	100	100
2	F	117/139 (84%)	116 (99%)	1 (1%)	0	100	100
All	All	1522/1701 (90%)	1487 (98%)	33 (2%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	332	TRP
1	B	226	ILE

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	255/361 (71%)	243 (95%)	12 (5%)	23	52
1	B	222/361 (62%)	219 (99%)	3 (1%)	59	73
1	C	273/361 (76%)	265 (97%)	8 (3%)	37	62
2	D	85/114 (75%)	84 (99%)	1 (1%)	63	75
2	E	88/114 (77%)	85 (97%)	3 (3%)	32	59
2	F	76/114 (67%)	74 (97%)	2 (3%)	40	64
All	All	999/1425 (70%)	970 (97%)	29 (3%)	37	62

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

Mol	Chain	Res	Type
1	A	8	ILE
1	A	34	VAL
1	A	50	LEU
1	A	226	ILE
1	A	238	GLU
1	A	254	GLU
1	A	273	ILE
1	A	297	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	298	LEU
1	A	357	VAL
1	A	389	VAL
1	A	418	CYS
1	B	34	VAL
1	B	202	LEU
1	B	315	VAL
1	C	8	ILE
1	C	34	VAL
1	C	35	LYS
1	C	65	CYS
1	C	127	LEU
1	C	185	LEU
1	C	243	GLU
1	C	385	MET
2	D	110	CYS
2	E	76	CYS
2	E	81	LYS
2	E	133	ILE
2	F	73	CYS
2	F	120	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	B	37	ASN
1	B	260	HIS
1	B	264	HIS
1	C	398	ASN
2	D	2	HIS
2	D	116	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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, 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	404/428 (94%)	0.88	52 (12%) 7 6	19, 39, 63, 86	0
1	B	394/428 (92%)	1.38	95 (24%) 2 1	31, 69, 93, 141	0
1	C	406/428 (94%)	0.91	51 (12%) 8 6	20, 40, 73, 90	0
2	D	124/139 (89%)	0.60	7 (5%) 30 20	20, 41, 62, 72	0
2	E	123/139 (88%)	0.75	11 (8%) 15 12	27, 55, 85, 102	0
2	F	121/139 (87%)	0.68	9 (7%) 20 15	35, 54, 70, 84	0
All	All	1572/1701 (92%)	0.96	225 (14%) 6 5	19, 48, 84, 141	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ASP	11.4
1	B	221	ASN	7.8
1	B	100	TYR	7.3
1	C	381	ASN	6.6
1	C	100	TYR	6.2
1	A	207	GLU	5.7
1	A	100	TYR	5.6
1	C	339	GLU	5.4
1	C	225	GLY	5.4
2	E	115	SER	5.4
1	B	29	ASP	5.4
1	B	14	ALA	5.3
1	B	228	GLY	5.2
1	B	207	GLU	5.2
1	B	204	GLN	5.2
1	B	153	GLU	5.0
1	B	206	GLU	5.0
1	A	257	PHE	4.9
1	B	208	VAL	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	220	ARG	4.8
1	A	417	PRO	4.8
1	A	269	MET	4.8
1	C	242	GLU	4.7
1	C	221	ASN	4.7
1	A	232	LYS	4.6
1	B	317	PHE	4.5
1	A	131	ASP	4.4
1	B	224	TYR	4.3
1	C	128	HIS	4.2
1	B	257	PHE	4.1
1	B	347	GLY	4.0
1	B	233	ALA	4.0
1	A	65	CYS	4.0
1	B	223	VAL	4.0
2	E	127	TYR	3.9
1	B	244	TYR	3.9
1	B	378	THR	3.8
1	C	11	ASP	3.8
1	B	181	MET	3.8
2	D	86	LYS	3.7
1	C	336	PRO	3.7
2	D	115	SER	3.7
1	C	237	ASN	3.7
2	D	75	ASN	3.6
2	E	75	ASN	3.6
1	B	101	ILE	3.6
1	B	214	HIS	3.6
1	B	222	GLY	3.6
1	B	412	VAL	3.6
1	B	131	ASP	3.6
1	B	418	CYS	3.6
1	B	48	ILE	3.6
1	A	395	LYS	3.5
1	C	38	ILE	3.5
1	B	5	TYR	3.5
1	A	344	ASP	3.5
1	B	118	PRO	3.5
1	B	230	TYR	3.5
1	A	225	GLY	3.5
1	B	328	ALA	3.4
1	B	6	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	325	ILE	3.4
1	C	224	TYR	3.4
1	B	12	HIS	3.4
1	B	213	THR	3.4
1	B	268	PHE	3.3
1	B	246	GLU	3.3
1	B	419	ILE	3.3
1	B	178	LEU	3.3
2	F	86	LYS	3.3
1	B	372	ALA	3.3
1	B	267	PRO	3.2
1	B	185	LEU	3.2
1	C	127	LEU	3.2
1	B	253	VAL	3.2
1	C	228	GLY	3.2
2	D	77	ASN	3.2
1	C	226	ILE	3.2
1	A	381	ASN	3.2
1	A	5	TYR	3.2
1	B	215	ILE	3.1
1	A	378	THR	3.1
1	C	394	GLU	3.1
1	C	246	GLU	3.1
1	A	129	MET	3.1
1	B	304	PHE	3.1
1	C	235	ASP	3.1
1	B	269	MET	3.0
1	A	415	TYR	3.0
1	C	155	GLY	3.0
1	C	129	MET	3.0
1	A	11	ASP	2.9
1	B	344	ASP	2.9
1	B	65	CYS	2.9
1	C	13	ILE	2.9
1	A	245	ARG	2.9
1	A	414	ALA	2.9
1	B	177	VAL	2.9
1	C	133	TYR	2.9
1	A	390	ARG	2.9
1	A	388	HIS	2.9
2	D	103	VAL	2.9
1	B	270	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	421	CYS	2.8
1	B	128	HIS	2.8
1	B	11	ASP	2.8
1	B	316	TYR	2.8
1	B	116	VAL	2.7
1	A	130	ILE	2.7
1	C	120	TYR	2.7
1	C	302	ASN	2.7
2	E	50	GLN	2.7
1	C	268	PHE	2.7
1	B	243	GLU	2.7
1	A	231	LEU	2.7
1	A	9	THR	2.7
1	B	311	ALA	2.7
1	C	205	TYR	2.7
1	A	228	GLY	2.6
2	E	102	GLU	2.6
1	A	389	VAL	2.6
1	A	393	ALA	2.6
1	B	326	ASP	2.6
1	A	78	GLU	2.6
2	F	28	ALA	2.6
1	B	349	SER	2.6
2	E	100	ILE	2.6
2	E	63	GLU	2.6
1	B	361	ALA	2.6
2	E	105	HIS	2.6
1	B	136	GLU	2.6
2	F	74	ARG	2.6
1	C	156	SER	2.5
1	B	298	LEU	2.5
1	B	318	THR	2.5
1	A	253	VAL	2.5
1	B	113	TYR	2.5
1	A	372	ALA	2.5
1	A	145	ASN	2.5
1	B	259	LYS	2.5
1	A	419	ILE	2.4
1	B	274	SER	2.4
1	C	355	ARG	2.4
1	C	240	PRO	2.4
1	A	122	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	116	HIS	2.4
1	C	9	THR	2.4
1	C	344	ASP	2.4
1	A	244	TYR	2.4
1	A	203	GLU	2.4
1	C	253	VAL	2.4
1	B	321	ALA	2.4
1	C	426	ALA	2.4
1	C	239	PHE	2.4
1	B	324	LEU	2.4
2	E	32	VAL	2.4
1	A	127	LEU	2.3
1	B	44	PHE	2.3
1	C	257	PHE	2.3
1	A	392	MET	2.3
1	B	205	TYR	2.3
1	B	241	SER	2.3
2	F	107	PHE	2.3
2	E	99	PHE	2.3
1	B	275	ARG	2.3
1	B	299	ARG	2.3
1	C	51	GLY	2.3
1	B	397	TYR	2.3
2	D	100	ILE	2.2
2	F	36	LEU	2.2
1	A	403	LYS	2.2
1	B	203	GLU	2.2
1	B	60	ILE	2.2
1	C	233	ALA	2.2
1	C	333	PRO	2.2
1	B	114	LEU	2.2
1	B	358	LEU	2.2
1	A	368	ARG	2.2
1	C	334	ILE	2.2
2	F	100	ILE	2.2
1	B	45	PHE	2.2
1	B	196	PHE	2.2
1	C	415	TYR	2.2
1	A	217	VAL	2.2
1	B	212	ILE	2.2
1	B	313	GLU	2.2
1	B	381	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	44	PHE	2.2
2	F	80	TRP	2.2
1	C	213	THR	2.2
1	B	54	LEU	2.2
1	C	341	ALA	2.2
1	B	49	THR	2.1
1	B	84	ILE	2.1
1	C	198	LEU	2.1
1	A	66	SER	2.1
1	A	391	MET	2.1
1	B	258	ALA	2.1
1	B	286	ARG	2.1
1	B	296	ASP	2.1
2	F	120	VAL	2.1
1	B	297	LEU	2.1
1	A	97	GLU	2.1
1	C	380	PHE	2.1
2	E	16	ASP	2.1
1	C	21	GLY	2.1
2	D	99	PHE	2.1
1	C	143	LEU	2.1
1	A	213	THR	2.1
1	C	243	GLU	2.1
1	B	182	LYS	2.0
1	C	270	VAL	2.0
1	A	37	ASN	2.0
1	A	226	ILE	2.0
1	C	8	ILE	2.0
1	A	160	HIS	2.0
1	B	133	TYR	2.0
1	B	346	PHE	2.0
1	B	354	PRO	2.0
1	C	354	PRO	2.0
1	A	206	GLU	2.0
1	A	48	ILE	2.0
1	A	20	GLY	2.0
1	C	402	GLU	2.0
1	B	329	LEU	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 [i](#)

There are no oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
3	ZN	E	701	1/1	0.97	0.04	75,75,75,75	0
3	ZN	D	701	1/1	0.98	0.06	43,43,43,43	0
3	ZN	F	701	1/1	0.98	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.