



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 11:13 pm BST

PDB ID : 3IHP
Title : Covalent Ubiquitin-Usp5 Complex
Authors : Walker, J.R.; Avvakumov, G.V.; Xue, S.; Butler-Cole, C.; Weigelt, J.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2009-07-30
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

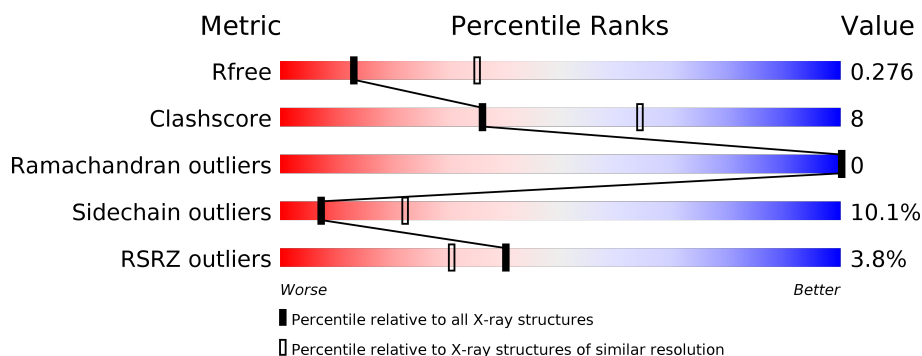
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	854	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>14%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	854	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>14%</div> <div>•</div> <div>20%</div> </div> </div>
2	C	75	<div> <div></div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>
2	D	75	<div> <div></div> <div> <div></div> <div>76%</div> <div>23%</div> <div>•</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11800 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 Ubiquitin carboxyl-terminal hydrolase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	3	0
			5265	3346	879	1005	35			
1	B	681	Total	C	N	O	S	0	0	0
			5300	3371	886	1009	34			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP P45974-2
A	-17	GLY	-	EXPRESSION TAG	UNP P45974-2
A	-16	SER	-	EXPRESSION TAG	UNP P45974-2
A	-15	SER	-	EXPRESSION TAG	UNP P45974-2
A	-14	HIS	-	EXPRESSION TAG	UNP P45974-2
A	-13	HIS	-	EXPRESSION TAG	UNP P45974-2
A	-12	HIS	-	EXPRESSION TAG	UNP P45974-2
A	-11	HIS	-	EXPRESSION TAG	UNP P45974-2
A	-10	HIS	-	EXPRESSION TAG	UNP P45974-2
A	-9	HIS	-	EXPRESSION TAG	UNP P45974-2
A	-8	SER	-	EXPRESSION TAG	UNP P45974-2
A	-7	SER	-	EXPRESSION TAG	UNP P45974-2
A	-6	GLY	-	EXPRESSION TAG	UNP P45974-2
A	-5	LEU	-	EXPRESSION TAG	UNP P45974-2
A	-4	VAL	-	EXPRESSION TAG	UNP P45974-2
A	-3	PRO	-	EXPRESSION TAG	UNP P45974-2
A	-2	ARG	-	EXPRESSION TAG	UNP P45974-2
A	-1	GLY	-	EXPRESSION TAG	UNP P45974-2
A	0	SER	-	EXPRESSION TAG	UNP P45974-2
B	-18	MET	-	EXPRESSION TAG	UNP P45974-2
B	-17	GLY	-	EXPRESSION TAG	UNP P45974-2
B	-16	SER	-	EXPRESSION TAG	UNP P45974-2
B	-15	SER	-	EXPRESSION TAG	UNP P45974-2
B	-14	HIS	-	EXPRESSION TAG	UNP P45974-2
B	-13	HIS	-	EXPRESSION TAG	UNP P45974-2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	EXPRESSION TAG	UNP P45974-2
B	-11	HIS	-	EXPRESSION TAG	UNP P45974-2
B	-10	HIS	-	EXPRESSION TAG	UNP P45974-2
B	-9	HIS	-	EXPRESSION TAG	UNP P45974-2
B	-8	SER	-	EXPRESSION TAG	UNP P45974-2
B	-7	SER	-	EXPRESSION TAG	UNP P45974-2
B	-6	GLY	-	EXPRESSION TAG	UNP P45974-2
B	-5	LEU	-	EXPRESSION TAG	UNP P45974-2
B	-4	VAL	-	EXPRESSION TAG	UNP P45974-2
B	-3	PRO	-	EXPRESSION TAG	UNP P45974-2
B	-2	ARG	-	EXPRESSION TAG	UNP P45974-2
B	-1	GLY	-	EXPRESSION TAG	UNP P45974-2
B	0	SER	-	EXPRESSION TAG	UNP P45974-2

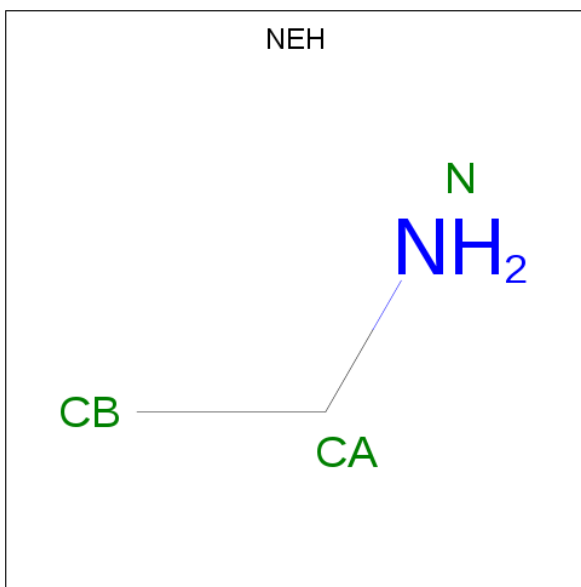
- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	D	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ETHANAMINE (three-letter code: NEH) (formula: C₂H₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	N	0	0
			3	2	1		
4	D	1	Total	C	N	0	0
			3	2	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

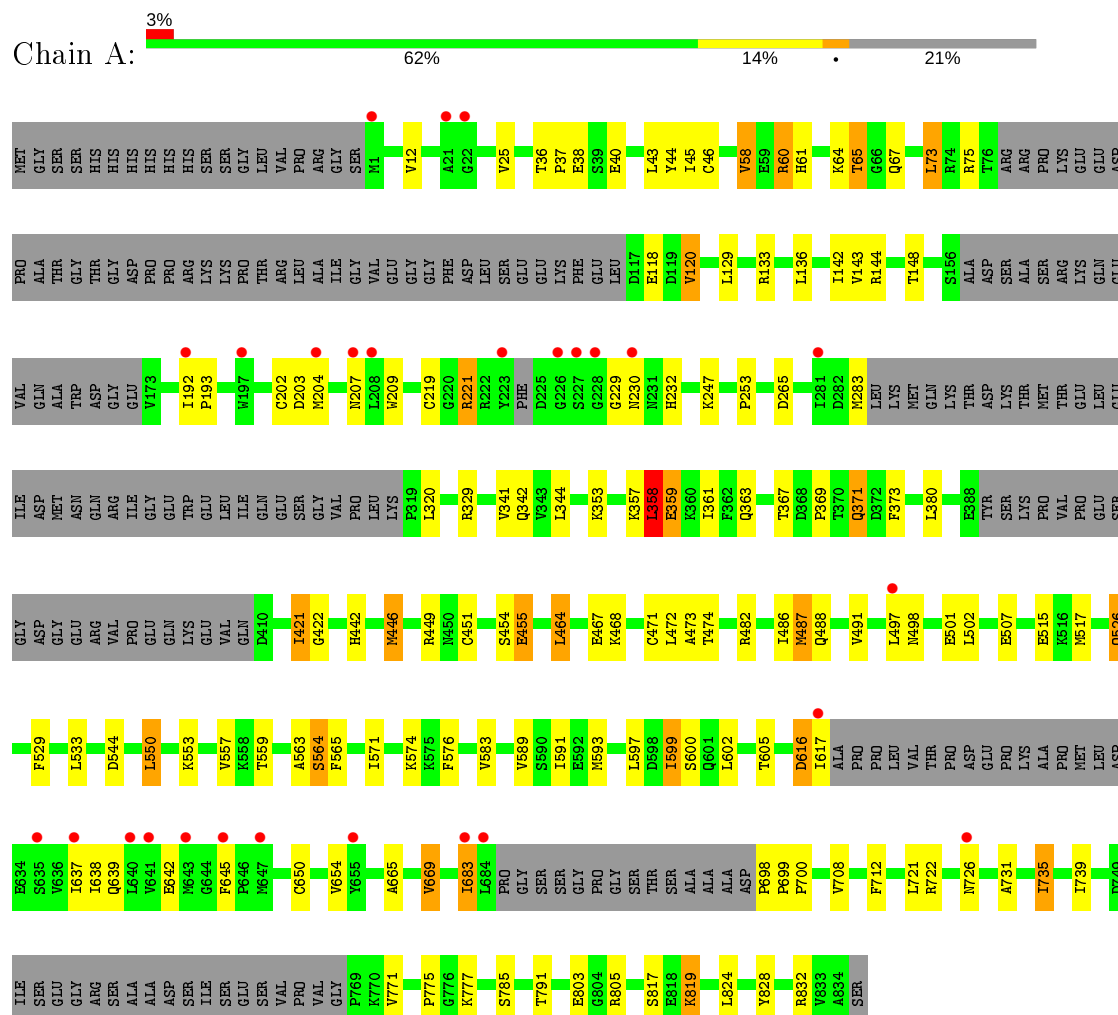
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	10	Total	O	0	0
			10	10		
6	C	2	Total	O	0	0
			2	2		

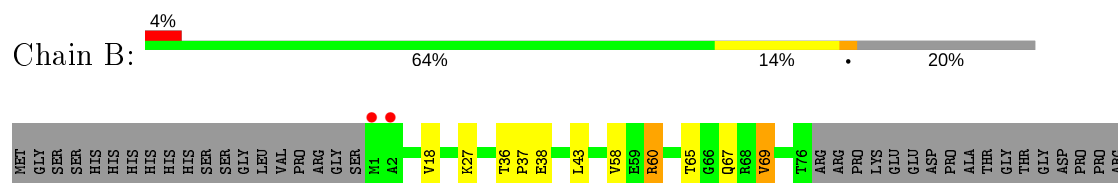
3 Residue-property plots

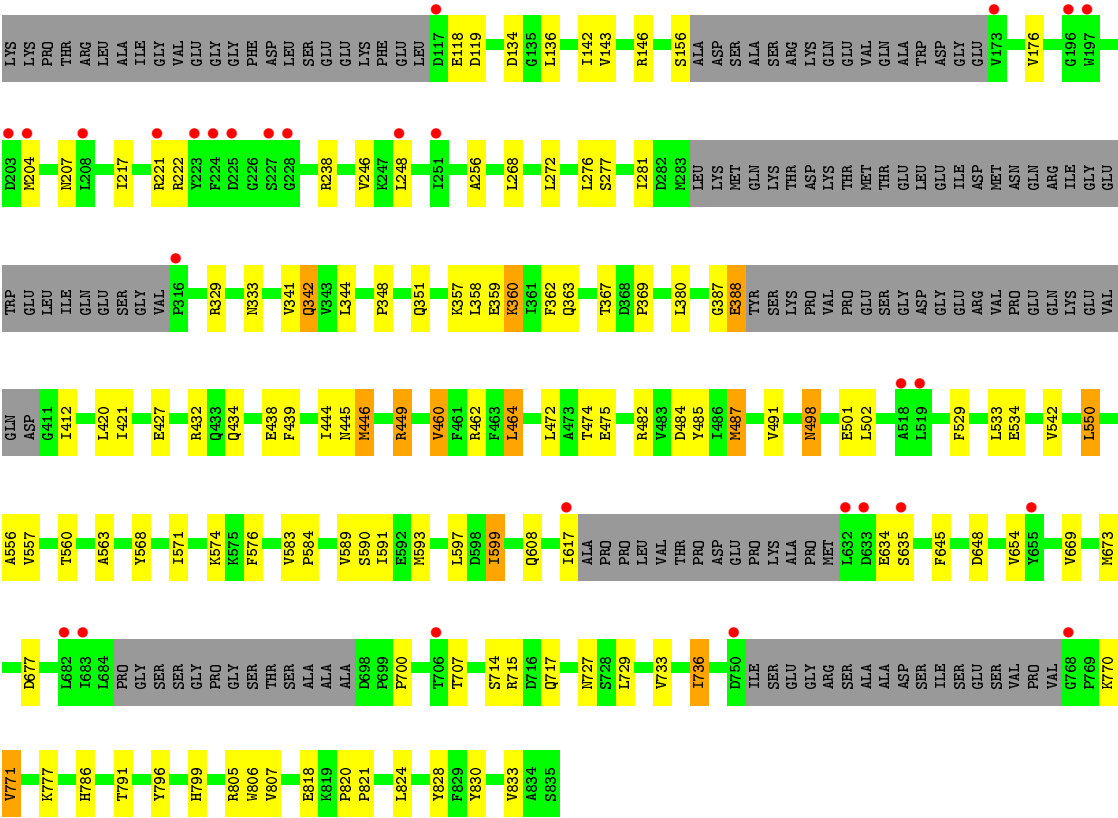
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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: Ubiquitin carboxyl-terminal hydrolase 5

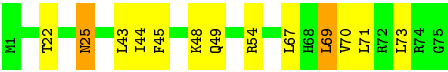
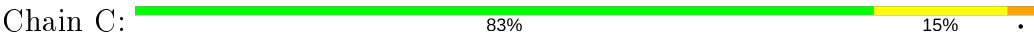


- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 5





● Molecule 2: Ubiquitin



● Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.30Å 188.84Å 207.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 2.80 34.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.90-2.80) 98.0 (34.90-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.224 , 0.276 0.229 , 0.276	Depositor DCC
R_{free} test set	3298 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11800	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, NEH, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	1/5381 (0.0%)	0.64	1/7293 (0.0%)
1	B	0.55	1/5419 (0.0%)	0.65	1/7346 (0.0%)
2	C	0.49	0/603	0.66	0/811
2	D	0.51	0/603	0.68	0/811
All	All	0.54	2/12006 (0.0%)	0.65	2/16261 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	715	ARG	NE-CZ	6.72	1.41	1.33
1	A	455	GLU	CG-CD	5.22	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	715	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	358	LEU	CA-CB-CG	5.18	127.22	115.30

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	5265	0	5039	95	0
1	B	5300	0	5085	76	0
2	C	597	0	626	7	0
2	D	597	0	626	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	C	3	0	4	0	0
4	D	3	0	3	0	0
5	D	1	0	0	0	0
6	A	20	0	0	1	0
6	B	10	0	0	0	0
6	C	2	0	0	0	0
All	All	11800	0	11383	185	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 8.

All (185) 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:221:ARG:HD2	1:A:221:ARG:H	1.03	1.09
1:A:221:ARG:HD2	1:A:221:ARG:N	1.76	0.98
1:A:819:LYS:HD3	1:A:819:LYS:H	1.32	0.94
1:B:360:LYS:H	1:B:360:LYS:HE3	1.40	0.84
1:A:468:LYS:HB3	1:A:559:THR:HG22	1.59	0.84
1:B:36:THR:HG22	1:B:38:GLU:H	1.44	0.83
1:A:221:ARG:CD	1:A:221:ARG:H	1.93	0.78
1:A:36:THR:HG22	1:A:38:GLU:H	1.49	0.78
1:A:202:CYS:HB3	1:A:232:HIS:HE1	1.52	0.75
1:A:75:ARG:HG2	1:A:118:GLU:HB3	1.69	0.75
1:B:427:GLU:HG3	1:B:434:GLN:NE2	2.05	0.71
1:B:818:GLU:O	1:B:820:PRO:HD3	1.92	0.70
1:B:60:ARG:CG	1:B:60:ARG:HH11	2.05	0.69
1:A:591:ILE:HG22	1:A:593:MET:HE3	1.75	0.69
1:B:498:ASN:HD22	1:B:498:ASN:H	1.40	0.68
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.07	0.68
1:A:529:PHE:HD1	1:A:593:MET:HE1	1.60	0.67
1:A:253:PRO:HA	1:A:283:MET:HB3	1.77	0.67
1:A:819:LYS:N	1:A:819:LYS:HD3	2.07	0.66
1:B:421:ILE:HB	1:B:446:MET:HE1	1.77	0.66
1:A:593:MET:HG3	1:A:828:TYR:CZ	2.31	0.66
1:A:529:PHE:CD1	1:A:593:MET:CE	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HD11	1:A:73:LEU:HD22	1.77	0.65
1:A:449:ARG:HH22	2:C:48:LYS:HZ1	1.43	0.65
1:A:529:PHE:CD1	1:A:593:MET:HE2	2.31	0.65
1:B:333:ASN:HD22	1:B:432:ARG:HA	1.62	0.64
1:A:529:PHE:HD1	1:A:593:MET:CE	2.11	0.63
1:A:638:ILE:O	1:A:642:GLU:HG2	1.98	0.63
1:A:473:ALA:HB3	1:A:550:LEU:HD21	1.81	0.63
2:D:7:THR:HG22	2:D:9:THR:H	1.64	0.62
1:A:497:LEU:HD12	1:A:526:GLN:HE22	1.65	0.61
1:A:421:ILE:O	1:A:442:HIS:HE1	1.82	0.61
1:B:387:GLY:O	1:B:388:GLU:HB3	2.01	0.61
1:B:634:GLU:HG2	1:B:635:SER:H	1.66	0.61
1:A:65:THR:HG22	1:A:67:GLN:H	1.66	0.60
1:A:817:SER:HB2	1:A:819:LYS:NZ	2.16	0.60
1:B:359:GLU:O	1:B:363:GLN:HG2	2.01	0.60
2:D:43:LEU:HD23	2:D:69:LEU:HD13	1.83	0.60
1:A:37:PRO:HD3	1:A:43:LEU:HD22	1.83	0.59
1:B:591:ILE:HG22	1:B:593:MET:HE3	1.83	0.59
1:A:421:ILE:HB	1:A:446:MET:HE1	1.83	0.59
1:A:468:LYS:HB3	1:A:559:THR:CG2	2.31	0.59
1:A:593:MET:HG3	1:A:828:TYR:CE2	2.38	0.59
1:A:486:ILE:HG13	1:A:486:ILE:O	2.03	0.58
1:B:176:VAL:HG12	1:B:268:LEU:HB2	1.86	0.57
1:A:464:LEU:HD13	1:A:771:VAL:HG11	1.86	0.57
2:C:44:ILE:HD13	2:C:70:VAL:HG22	1.86	0.57
1:B:60:ARG:HG2	1:B:60:ARG:HH11	1.69	0.57
1:A:488:GLN:HB3	1:A:574:LYS:HD2	1.87	0.57
1:A:371:GLN:HA	1:A:371:GLN:OE1	2.06	0.56
1:A:421:ILE:C	1:A:421:ILE:HD13	2.27	0.55
1:B:464:LEU:HD22	1:B:771:VAL:HG21	1.87	0.54
1:B:445:ASN:O	1:B:449:ARG:HD2	2.08	0.54
2:C:22:THR:OG1	2:C:25:ASN:HB2	2.08	0.54
1:B:348:PRO:HA	1:B:351:GLN:HE21	1.73	0.54
1:B:445:ASN:HB3	1:B:449:ARG:NH2	2.23	0.54
1:A:202:CYS:HB3	1:A:232:HIS:CE1	2.39	0.53
1:A:358:LEU:HD12	1:A:358:LEU:C	2.28	0.53
1:A:497:LEU:HD12	1:A:526:GLN:NE2	2.23	0.53
1:B:634:GLU:HG2	1:B:635:SER:N	2.23	0.52
1:A:358:LEU:HD12	1:A:359:GLU:N	2.24	0.52
1:B:474:THR:CG2	1:B:550:LEU:HD13	2.39	0.52
1:B:593:MET:HG3	1:B:828:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ILE:HD13	1:A:422:GLY:N	2.25	0.52
1:A:36:THR:HG23	1:A:37:PRO:HD2	1.92	0.52
1:A:464:LEU:HB3	1:A:563:ALA:HB3	1.92	0.52
1:B:36:THR:HG23	1:B:37:PRO:HD2	1.92	0.51
1:A:209:TRP:CZ3	1:A:247:LYS:HB2	2.45	0.51
1:B:217:ILE:HG12	1:B:248:LEU:HD11	1.91	0.51
1:B:464:LEU:HB3	1:B:563:ALA:HB3	1.91	0.51
1:A:421:ILE:HB	1:A:446:MET:CE	2.42	0.50
1:A:472:LEU:HD22	1:A:557:VAL:HG23	1.93	0.50
1:B:533:LEU:HD21	1:B:599:ILE:HD11	1.92	0.50
1:A:487:MET:HG2	1:A:571:ILE:HG12	1.93	0.50
1:B:427:GLU:HG3	1:B:434:GLN:CD	2.31	0.50
1:B:484:ASP:OD1	1:B:485:TYR:N	2.37	0.50
1:B:367:THR:O	1:B:369:PRO:HD3	2.12	0.49
1:A:136:LEU:HB3	1:A:144:ARG:HG2	1.94	0.49
1:A:367:THR:O	1:A:369:PRO:HD3	2.13	0.49
1:B:421:ILE:HD13	1:B:439:PHE:HE1	1.77	0.49
1:A:449:ARG:HH21	1:A:449:ARG:HG3	1.77	0.48
1:B:591:ILE:CG2	1:B:593:MET:HE3	2.42	0.48
1:B:645:PHE:HD1	1:B:673:MET:CE	2.25	0.48
1:B:221:ARG:HG2	1:B:222:ARG:N	2.29	0.48
1:B:472:LEU:HD13	1:B:557:VAL:CG2	2.44	0.48
1:B:60:ARG:CG	1:B:60:ARG:NH1	2.71	0.48
2:C:43:LEU:CD2	2:C:69:LEU:HD13	2.44	0.48
1:A:498:ASN:HB2	1:A:501:GLU:HB2	1.94	0.48
1:A:60:ARG:CG	1:A:60:ARG:NH1	2.72	0.48
1:A:565:PHE:CE2	1:A:599:ILE:HG23	2.49	0.47
1:A:817:SER:HB2	1:A:819:LYS:HZ3	1.79	0.47
1:A:473:ALA:CB	1:A:550:LEU:HD21	2.44	0.47
1:B:501:GLU:OE1	1:B:501:GLU:N	2.45	0.47
1:A:731:ALA:O	1:A:735:ILE:HG13	2.15	0.47
1:B:67:GLN:NE2	1:B:69:VAL:HG23	2.30	0.47
1:B:645:PHE:HD1	1:B:673:MET:HE1	1.79	0.47
1:B:438:GLU:HB2	2:D:42:ARG:NH2	2.30	0.47
1:A:482:ARG:HD3	6:A:838:HOH:O	2.15	0.46
2:D:43:LEU:CD2	2:D:69:LEU:HD13	2.45	0.46
1:B:358:LEU:HD21	1:B:362:PHE:CE2	2.50	0.46
1:A:204:MET:SD	1:A:229:GLY:HA2	2.56	0.46
1:B:714:SER:H	1:B:717:GLN:NE2	2.14	0.46
1:A:353:LYS:HE2	1:A:451:CYS:SG	2.55	0.46
1:A:638:ILE:HG13	1:A:639:GLN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLU:HB3	1:A:517:MET:HG3	1.98	0.45
1:B:820:PRO:HA	1:B:821:PRO:HD3	1.75	0.45
1:A:40:GLU:OE1	1:A:40:GLU:N	2.49	0.45
1:A:735:ILE:HG13	1:A:735:ILE:H	1.46	0.45
2:D:23:ILE:HG12	2:D:50:LEU:HB3	1.97	0.45
1:A:591:ILE:CG2	1:A:593:MET:HE3	2.43	0.45
2:C:43:LEU:C	2:C:44:ILE:HD12	2.38	0.45
1:B:276:LEU:HB3	1:B:281:ILE:HB	1.99	0.45
1:B:427:GLU:HG3	1:B:434:GLN:HE22	1.80	0.45
1:A:202:CYS:SG	1:A:203:ASP:N	2.90	0.44
1:A:721:LEU:HB3	1:A:726:ASN:HD22	1.83	0.44
1:B:434:GLN:HA	1:B:434:GLN:OE1	2.17	0.44
1:A:544:ASP:OD1	1:A:553:LYS:HD2	2.17	0.44
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.32	0.44
1:A:637:ILE:HG13	1:A:654:VAL:HG21	2.00	0.44
1:B:568:TYR:HA	1:B:830:TYR:O	2.17	0.44
1:B:584:PRO:HB3	2:D:71:LEU:HD13	1.99	0.44
1:A:474:THR:CG2	1:A:550:LEU:HD13	2.48	0.44
1:B:529:PHE:CD1	1:B:593:MET:CE	3.01	0.44
1:B:498:ASN:N	1:B:498:ASN:HD22	2.05	0.44
1:B:445:ASN:HB3	1:B:449:ARG:HH21	1.83	0.44
1:B:589:VAL:CG1	1:B:590:SER:N	2.81	0.44
1:B:589:VAL:HG12	1:B:590:SER:N	2.31	0.44
1:A:60:ARG:HH11	1:A:60:ARG:HG3	1.81	0.43
1:B:333:ASN:ND2	1:B:432:ARG:HA	2.32	0.43
1:A:120:VAL:HG22	1:A:133:ARG:HD2	2.00	0.43
1:A:357:LYS:O	1:A:361:ILE:HG13	2.18	0.43
1:A:645:PHE:HB2	1:A:650:CYS:SG	2.57	0.43
1:B:460:VAL:HG22	1:B:568:TYR:HD2	1.83	0.43
1:B:593:MET:HG3	1:B:828:TYR:CE2	2.53	0.43
1:B:487:MET:HG2	1:B:571:ILE:HG12	2.00	0.43
1:B:474:THR:O	1:B:475:GLU:HB2	2.17	0.43
1:B:805:ARG:HG2	1:B:806:TRP:N	2.34	0.43
1:B:799:HIS:HA	1:B:807:VAL:O	2.19	0.43
1:A:44:TYR:CD2	1:A:58:VAL:HG21	2.54	0.43
1:A:600:SER:C	1:A:602:LEU:H	2.22	0.43
2:D:7:THR:HG22	2:D:8:LEU:N	2.33	0.43
1:A:698:PRO:HA	1:A:699:PRO:HD3	1.67	0.43
1:A:464:LEU:HD22	1:A:771:VAL:HG21	2.01	0.43
1:A:464:LEU:HB2	1:A:564:SER:HB3	2.01	0.42
1:B:498:ASN:H	1:B:498:ASN:ND2	2.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ARG:NH2	1:B:359:GLU:OE1	2.52	0.42
2:D:22:THR:OG1	2:D:25:ASN:HB2	2.19	0.42
1:B:37:PRO:HD3	1:B:43:LEU:HD22	2.01	0.42
2:C:44:ILE:HD13	2:C:70:VAL:CG2	2.49	0.42
1:B:529:PHE:CD1	1:B:593:MET:HE2	2.55	0.42
1:A:358:LEU:CD1	1:A:358:LEU:C	2.88	0.42
1:A:61:HIS:O	1:A:65:THR:HB	2.19	0.42
1:A:683:ILE:H	1:A:683:ILE:HG13	1.61	0.42
1:B:472:LEU:HD13	1:B:557:VAL:HG21	2.01	0.42
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.82	0.41
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.77	0.41
1:A:371:GLN:CA	1:A:371:GLN:OE1	2.68	0.41
1:A:373:PHE:CE1	1:A:446:MET:HG2	2.55	0.41
1:A:529:PHE:CD1	1:A:593:MET:HE1	2.44	0.41
1:B:134:ASP:N	1:B:134:ASP:OD2	2.53	0.41
1:B:60:ARG:HG3	1:B:60:ARG:HH11	1.84	0.41
1:A:358:LEU:HA	1:A:361:ILE:HD12	2.02	0.41
1:A:474:THR:HG23	1:A:550:LEU:HD13	2.03	0.41
1:B:357:LYS:HA	1:B:360:LYS:NZ	2.35	0.41
1:B:542:VAL:HB	1:B:556:ALA:HB3	2.02	0.41
1:B:700:PRO:HB3	1:B:727:ASN:ND2	2.35	0.41
1:B:256:ALA:HB3	1:B:272:LEU:HD21	2.02	0.41
1:B:733:VAL:HA	1:B:736:ILE:HD11	2.03	0.41
1:A:665:ALA:O	1:A:669:VAL:HG22	2.20	0.41
1:A:219:CYS:SG	1:A:230:ASN:N	2.86	0.41
1:A:699:PRO:HA	1:A:700:PRO:HD3	1.71	0.41
1:B:589:VAL:HG12	1:B:591:ILE:HG13	2.03	0.41
2:D:37:PRO:HA	2:D:38:PRO:HD3	1.90	0.41
1:B:342:GLN:HA	1:B:342:GLN:HE21	1.87	0.40
1:A:60:ARG:HH12	1:A:363:GLN:HG2	1.85	0.40
2:D:45:PHE:HB3	2:D:50:LEU:HD21	2.03	0.40
1:A:775:PRO:HD2	1:A:832:ARG:HD3	2.04	0.40
1:B:246:VAL:HG11	1:B:276:LEU:HD21	2.02	0.40
2:C:45:PHE:HB2	2:C:67:LEU:HD22	2.02	0.40
1:A:616:ASP:HB2	1:A:617:ILE:H	1.62	0.40
1:A:708:VAL:HG13	1:A:712:PHE:O	2.21	0.40
1:A:819:LYS:O	1:A:819:LYS:HG2	2.22	0.40
1:B:462:ARG:NH1	1:B:770:LYS:O	2.53	0.40
1:B:786:HIS:HB2	1:B:796:TYR:CE2	2.56	0.40
1:B:584:PRO:HG3	2:D:40:GLN:NE2	2.37	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	658/854 (77%)	629 (96%)	29 (4%)	0	100	100
1	B	665/854 (78%)	633 (95%)	32 (5%)	0	100	100
2	C	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
2	D	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
All	All	1469/1858 (79%)	1405 (96%)	64 (4%)	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	560/734 (76%)	501 (90%)	59 (10%)	7	20
1	B	564/734 (77%)	506 (90%)	58 (10%)	7	21
2	C	68/68 (100%)	62 (91%)	6 (9%)	10	29
2	D	68/68 (100%)	64 (94%)	4 (6%)	19	49
All	All	1260/1604 (79%)	1133 (90%)	127 (10%)	7	22

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	25	VAL

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Mol	Chain	Res	Type
1	A	46	CYS
1	A	58	VAL
1	A	60	ARG
1	A	64	LYS
1	A	65	THR
1	A	73	LEU
1	A	120	VAL
1	A	129	LEU
1	A	142	ILE
1	A	143	VAL
1	A	148	THR
1	A	207	ASN
1	A	221	ARG
1	A	265	ASP
1	A	320	LEU
1	A	329	ARG
1	A	341	VAL
1	A	342	GLN
1	A	344	LEU
1	A	358	LEU
1	A	359	GLU
1	A	371	GLN
1	A	380	LEU
1	A	421	ILE
1	A	446	MET
1	A	454	SER
1	A	455	GLU
1	A	464	LEU
1	A	467	GLU
1	A	471	CYS
1	A	487	MET
1	A	491	VAL
1	A	502	LEU
1	A	507	GLU
1	A	526	GLN
1	A	533	LEU
1	A	550	LEU
1	A	564	SER
1	A	576	PHE
1	A	583	VAL
1	A	589	VAL
1	A	597	LEU

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Mol	Chain	Res	Type
1	A	599	ILE
1	A	605	THR
1	A	616	ASP
1	A	669	VAL
1	A	683	ILE
1	A	722	ARG
1	A	735	ILE
1	A	739	ILE
1	A	777	LYS
1	A	785	SER
1	A	791	THR
1	A	803	GLU
1	A	805	ARG
1	A	819	LYS
1	A	824	LEU
1	B	18	VAL
1	B	27	LYS
1	B	58	VAL
1	B	60	ARG
1	B	65	THR
1	B	69	VAL
1	B	118	GLU
1	B	119	ASP
1	B	136	LEU
1	B	142	ILE
1	B	143	VAL
1	B	146	ARG
1	B	156	SER
1	B	204	MET
1	B	207	ASN
1	B	238	ARG
1	B	277	SER
1	B	329	ARG
1	B	341	VAL
1	B	342	GLN
1	B	344	LEU
1	B	360	LYS
1	B	380	LEU
1	B	388	GLU
1	B	412	ILE
1	B	420	LEU
1	B	444	ILE

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Mol	Chain	Res	Type
1	B	446	MET
1	B	449	ARG
1	B	460	VAL
1	B	464	LEU
1	B	482	ARG
1	B	487	MET
1	B	491	VAL
1	B	498	ASN
1	B	502	LEU
1	B	534	GLU
1	B	550	LEU
1	B	560	THR
1	B	574	LYS
1	B	576	PHE
1	B	583	VAL
1	B	597	LEU
1	B	599	ILE
1	B	608	GLN
1	B	617	ILE
1	B	648	ASP
1	B	654	VAL
1	B	669	VAL
1	B	677	ASP
1	B	707	THR
1	B	729	LEU
1	B	736	ILE
1	B	771	VAL
1	B	777	LYS
1	B	791	THR
1	B	824	LEU
1	B	833	VAL
2	C	25	ASN
2	C	49	GLN
2	C	54	ARG
2	C	69	LEU
2	C	71	LEU
2	C	73	LEU
2	D	24	GLU
2	D	48	LYS
2	D	60	ASN
2	D	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	342	GLN
1	A	442	HIS
1	A	526	GLN
1	A	551	GLN
1	A	608	GLN
1	A	667	ASN
1	A	726	ASN
1	B	61	HIS
1	B	63	ASN
1	B	333	ASN
1	B	342	GLN
1	B	351	GLN
1	B	498	ASN
1	B	608	GLN
1	B	667	ASN
1	B	672	HIS
1	B	717	GLN
1	B	727	ASN
2	D	40	GLN
2	D	60	ASN

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, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NEH	D	76	1,2	2,2,2	0.38	0	0,1,1	0.00	-
4	NEH	C	76	1,2	2,2,2	0.53	0	0,1,1	0.00	-

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	673/854 (78%)	-0.04	27 (4%) 38 28	47, 72, 107, 152	0
1	B	681/854 (79%)	0.01	30 (4%) 34 24	45, 70, 116, 159	0
2	C	75/75 (100%)	-0.25	0 100 100	49, 65, 84, 92	0
2	D	75/75 (100%)	-0.10	0 100 100	50, 65, 80, 84	0
All	All	1504/1858 (80%)	-0.03	57 (3%) 40 30	45, 70, 109, 159	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	633	ASP	5.4
1	B	224	PHE	5.4
1	B	225	ASP	4.8
1	B	632	LEU	4.3
1	B	768	GLY	4.3
1	B	173	VAL	4.2
1	B	1	MET	4.0
1	B	683	ILE	3.9
1	A	635	SER	3.6
1	B	117	ASP	3.6
1	A	230	ASN	3.5
1	B	617	ILE	3.4
1	B	251	ILE	3.3
1	A	192	ILE	3.3
1	A	1	MET	3.2
1	A	227	SER	3.2
1	B	682	LEU	3.1
1	A	683	ILE	3.1
1	A	617	ILE	3.0
1	A	647	MET	3.0
1	B	2	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	655	TYR	2.8
1	B	208	LEU	2.8
1	B	223	TYR	2.8
1	B	228	GLY	2.7
1	A	643	MET	2.7
1	B	750	ASP	2.6
1	A	22	GLY	2.5
1	A	645	PHE	2.5
1	A	197	TRP	2.5
1	A	228	GLY	2.5
1	A	684	LEU	2.5
1	A	655	TYR	2.4
1	A	21	ALA	2.4
1	B	227	SER	2.4
1	B	196	GLY	2.3
1	B	518	ALA	2.3
1	A	726	ASN	2.3
1	A	637	ILE	2.3
1	B	203	ASP	2.3
1	B	197	TRP	2.3
1	A	208	LEU	2.2
1	A	641	VAL	2.2
1	A	204	MET	2.2
1	A	497	LEU	2.2
1	A	226	GLY	2.2
1	B	519	LEU	2.2
1	A	281	ILE	2.2
1	B	248	LEU	2.1
1	B	316	PRO	2.1
1	A	223	TYR	2.1
1	B	221	ARG	2.1
1	B	204	MET	2.1
1	A	207	ASN	2.0
1	A	640	LEU	2.0
1	B	635	SER	2.0
1	B	706	THR	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 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. 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(\AA^2)	Q<0.9
3	ZN	B	836	1/1	0.86	0.06	94,94,94,94	0
5	CL	D	77	1/1	0.90	0.21	84,84,84,84	0
4	NEH	D	76	3/3	0.94	0.21	37,37,37,37	0
4	NEH	C	76	3/3	0.98	0.14	36,36,38,39	0
3	ZN	A	836	1/1	0.99	0.05	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.