



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:33 PM UTC

PDB ID : 3IHP / pdb_00003ihp
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

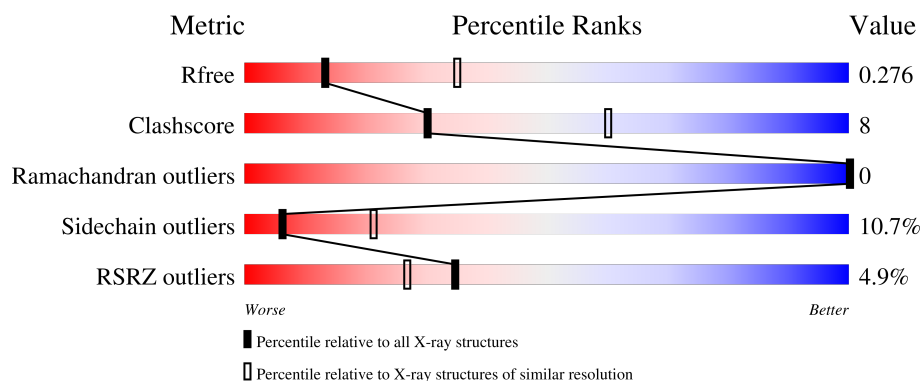
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	854	3% 61% 15% 21%
1	B	854	6% 63% 15% 20%
2	C	75	83% 16%
2	D	75	77% 20%

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

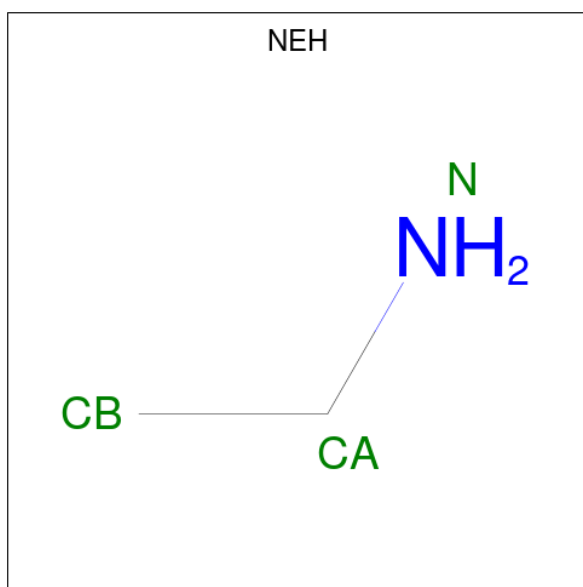
- Molecule 2 is a protein called Ubiquitin.

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is ETHANAMINE (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

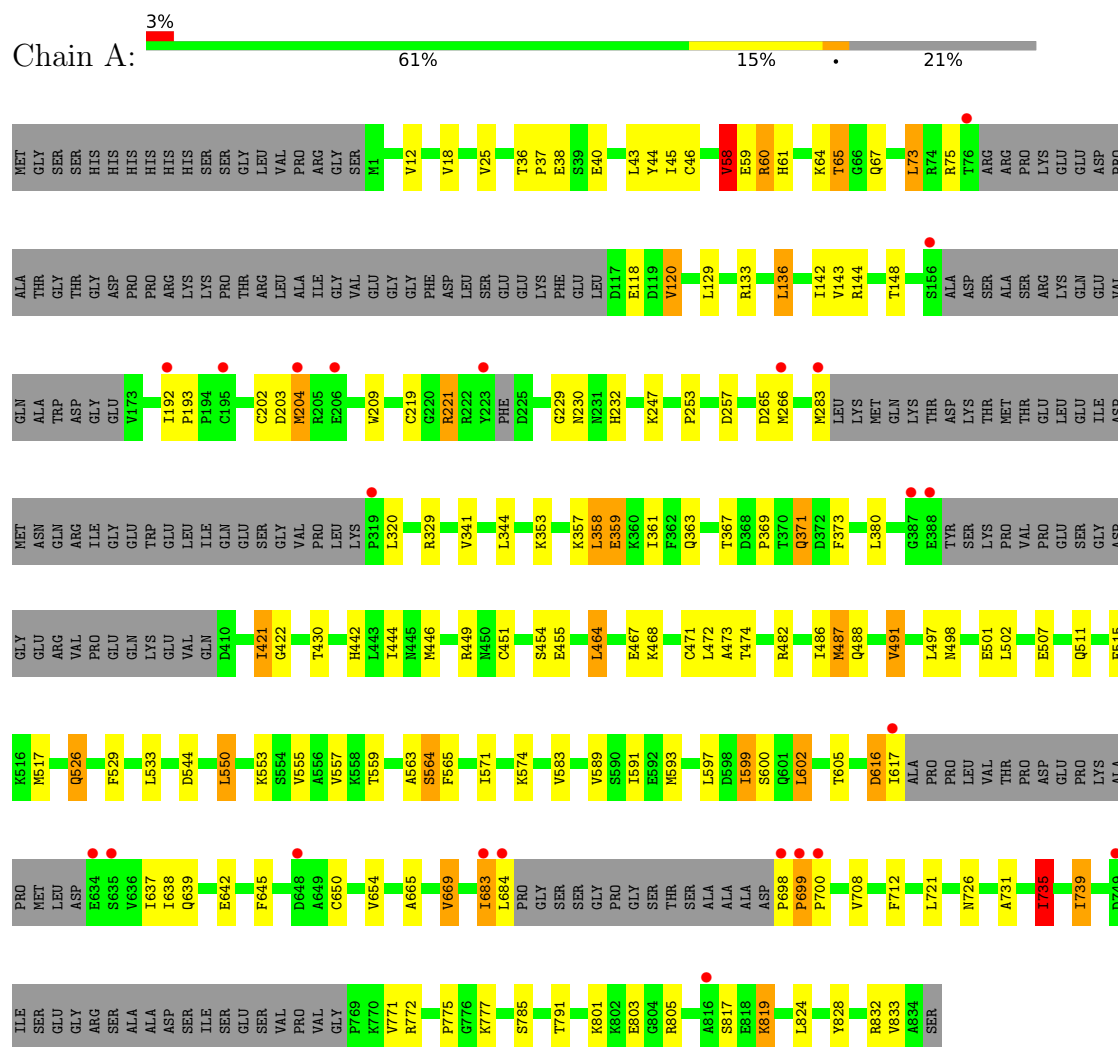
- Molecule 6 is water.

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		

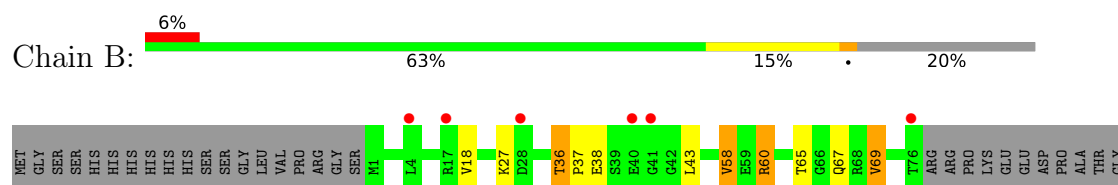
3 Residue-property plots [i](#)

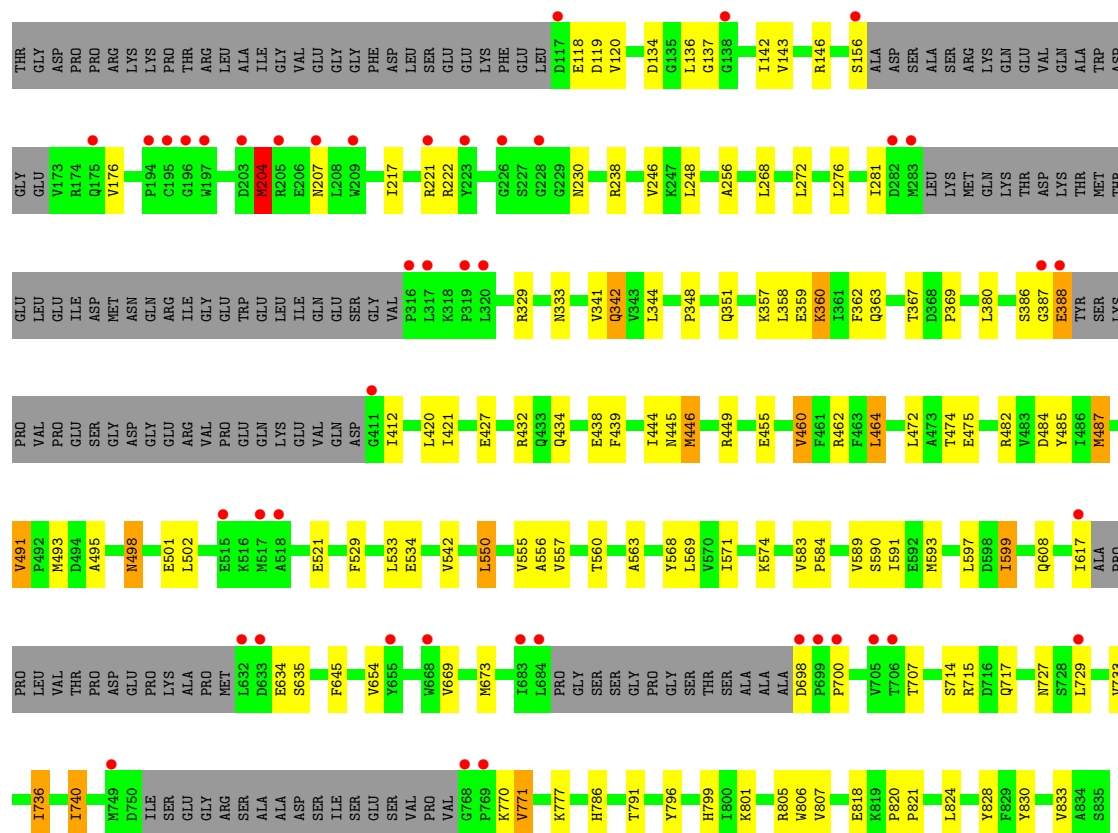
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ubiquitin carboxyl-terminal hydrolase 5



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 5





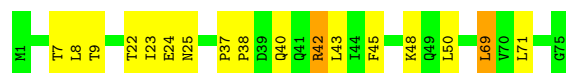
• Molecule 2: Ubiquitin

Chain C: 83% 16%



• Molecule 2: Ubiquitin

Chain D: 77% 20%



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	3371 reflections (5.02%)	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)	0.31 , 51.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NEH, ZN, 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	0.63	1/5381 (0.0%)	0.91	6/7293 (0.1%)
1	B	0.67	1/5419 (0.0%)	0.95	8/7346 (0.1%)
2	C	0.61	0/603	0.86	1/811 (0.1%)
2	D	0.63	0/603	0.91	0/811
All	All	0.65	2/12006 (0.0%)	0.93	15/16261 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	715	ARG	NE-CZ	7.94	1.41	1.33
1	A	491	VAL	CA-CB	6.19	1.59	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	VAL	CB-CA-C	-6.26	103.84	112.04
1	B	204	MET	N-CA-C	6.17	118.26	110.24
1	A	735	ILE	CB-CA-C	-5.93	104.04	112.22
1	B	698	ASP	CA-C-N	5.92	123.98	119.66
1	B	698	ASP	C-N-CA	5.92	123.98	119.66
1	A	739	ILE	CB-CA-C	-5.83	104.42	111.88
1	B	386	SER	N-CA-C	5.65	113.41	108.78
1	B	58	VAL	CB-CA-C	-5.65	104.52	112.14
1	A	491	VAL	CB-CA-C	5.45	116.26	111.08
1	B	137	GLY	N-CA-C	5.39	119.20	112.73
1	B	740	ILE	N-CA-CB	5.32	116.41	110.51
1	A	699	PRO	CA-C-N	5.18	126.32	119.84
1	A	699	PRO	C-N-CA	5.18	126.32	119.84
1	B	491	VAL	CB-CA-C	5.15	115.97	111.08
2	C	10	GLY	N-CA-C	-5.12	108.10	113.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5265	0	5039	98	0
1	B	5300	0	5085	82	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	194	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 (194) 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:A:529:PHE:HD1	1:A:593:MET:HE1	1.38	0.87
1:B:360:LYS:HE3	1:B:360:LYS:H	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:529:PHE:CD1	1:A:593:MET:HE1	2.17	0.78
1:A:221:ARG:H	1:A:221:ARG:CD	1.93	0.78
1:A:36:THR:HG22	1:A:38:GLU:H	1.49	0.78
1:A:75:ARG:HG2	1:A:118:GLU:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:CYS:HB3	1:A:232:HIS:HE1	1.52	0.75
1:A:449:ARG:HH22	2:C:48:LYS:HZ1	1.35	0.73
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:B:498:ASN:H	1:B:498:ASN:HD22	1.40	0.68
1:A:60:ARG:CG	1:A:60:ARG:HH11	2.07	0.68
1:A:253:PRO:HA	1:A:283:MET:HB3	1.77	0.67
1:A:819:LYS:HD3	1:A:819:LYS:N	2.07	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
1:A:45:ILE:HD11	1:A:73:LEU:HD22	1.77	0.65
1:A:591:ILE:HG22	1:A:593:MET:HE3	1.80	0.64
1:B:333:ASN:HD22	1:B:432:ARG:HA	1.62	0.64
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:634:GLU:HG2	1:B:635:SER:H	1.66	0.61
1:B:204:MET:HE1	1:B:230:ASN:OD1	2.00	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
1:B:529:PHE:CD1	1:B:593:MET:HE1	2.36	0.60
2:D:43:LEU:HD23	2:D:69:LEU:HD13	1.83	0.60
1:A:529:PHE:HD1	1:A:593:MET:CE	2.11	0.60
1:B:421:ILE:HB	1:B:446:MET:HE1	1.82	0.60
1:A:421:ILE:C	1:A:421:ILE:HD13	2.27	0.60
1:A:37:PRO:HD3	1:A:43:LEU:HD22	1.83	0.59
1:B:387:GLY:O	1:B:388:GLU:HB3	2.01	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:O	1:A:486:ILE:HG13	2.03	0.58
1:A:358:LEU:C	1:A:358:LEU:HD12	2.28	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:HH11	1:B:60:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:SER:HB2	1:A:819:LYS:HZ3	1.70	0.55
1:B:427:GLU:HG3	1:B:434:GLN:CD	2.31	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
1:A:591:ILE:CG2	1:A:593:MET:HE3	2.37	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:B:529:PHE:HD1	1:B:593:MET:HE1	1.74	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
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:A:257:ASP:HB3	1:A:266:MET:HE1	1.92	0.51
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:484:ASP:OD1	1:B:485:TYR:N	2.37	0.50
2:C:43:LEU:C	2:C:44:ILE:HD12	2.38	0.49
1:B:367:THR:O	1:B:369:PRO:HD3	2.12	0.49
1:B:591:ILE:HG22	1:B:593:MET:HE3	1.94	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:HG3	1:A:449:ARG:HH21	1.77	0.48
1:B:591:ILE:CG2	1:B:593:MET:HE3	2.43	0.48
1:B:645:PHE:HD1	1:B:673:MET:CE	2.25	0.48
1:A:600:SER:C	1:A:602:LEU:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:LEU:CD2	2:C:69:LEU:HD13	2.44	0.48
1:A:60:ARG:CG	1:A:60:ARG:NH1	2.72	0.48
1:A:498:ASN:HB2	1:A:501:GLU:HB2	1.94	0.48
1:A:565:PHE:CE2	1:A:599:ILE:HG23	2.49	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:A:358:LEU:C	1:A:358:LEU:CD1	2.88	0.47
1:A:593:MET:HA	1:A:593:MET:HE2	1.97	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
1:A:515:GLU:HB3	1:A:517:MET:HG3	1.98	0.45
1:B:487:MET:HE2	1:B:569:LEU:HD21	1.97	0.45
1:B:820:PRO:HA	1:B:821:PRO:HD3	1.75	0.45
1:A:40:GLU:N	1:A:40:GLU:OE1	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: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:60:ARG:NH1	1:A:60:ARG:HG3	2.32	0.44
1:A:544:ASP:OD1	1:A:553:LYS:HD2	2.17	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:421:ILE:HD12	1:B:421:ILE:C	2.43	0.44
1:B:529:PHE:CD1	1:B:593:MET:CE	3.01	0.44
1:B:498:ASN:HD22	1:B:498:ASN:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HH11	1:A:60:ARG:HG3	1.81	0.43
1:A:600:SER:C	1:A:602:LEU:N	2.75	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:493:MET:C	1:B:495:ALA:H	2.27	0.43
1:B:474:THR:O	1:B:475:GLU:HB2	2.17	0.43
1:A:421:ILE:HB	1:A:446:MET:HE1	2.01	0.43
1:B:357:LYS:NZ	1:B:455:GLU:OE2	2.42	0.43
1:B:799:HIS:HA	1:B:807:VAL:O	2.19	0.43
1:B:805:ARG:HG2	1:B:806:TRP:N	2.34	0.43
1:A:44:TYR:CD2	1:A:58:VAL:HG21	2.54	0.43
2:D:7:THR:HG22	2:D:8:LEU:N	2.33	0.43
1:A:464:LEU:HD22	1:A:771:VAL:HG21	2.01	0.43
1:A:698:PRO:HA	1:A:699:PRO:HD3	1.67	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
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: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:B:645:PHE:HD1	1:B:673:MET:HE1	1.84	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:OE1	1:A:371:GLN:CA	2.68	0.41
1:A:373:PHE:CE1	1:A:446:MET:HG2	2.55	0.41
1:A:442:HIS:CE1	1:A:446:MET:HE1	2.56	0.41
1:B:60:ARG:HH11	1:B:60:ARG:HG3	1.84	0.41
1:B:134:ASP:OD2	1:B:134:ASP:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:584:PRO:HG3	2:D:40:GLN:NE2	2.37	0.40
1:B:786:HIS:HB2	1:B:796:TYR:CE2	2.56	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%)	493 (88%)	67 (12%)	5	17
1	B	564/734 (77%)	505 (90%)	59 (10%)	6	22
2	C	68/68 (100%)	64 (94%)	4 (6%)	18	48
2	D	68/68 (100%)	64 (94%)	4 (6%)	18	48
All	All	1260/1604 (79%)	1126 (89%)	134 (11%)	6	22

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	18	VAL
1	A	25	VAL
1	A	46	CYS
1	A	58	VAL
1	A	59	GLU
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	136	LEU
1	A	142	ILE
1	A	143	VAL
1	A	148	THR
1	A	204	MET
1	A	221	ARG
1	A	265	ASP
1	A	320	LEU
1	A	329	ARG
1	A	341	VAL

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Mol	Chain	Res	Type
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	430	THR
1	A	444	ILE
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	511	GLN
1	A	526	GLN
1	A	533	LEU
1	A	550	LEU
1	A	555	VAL
1	A	564	SER
1	A	583	VAL
1	A	589	VAL
1	A	597	LEU
1	A	599	ILE
1	A	602	LEU
1	A	605	THR
1	A	616	ASP
1	A	669	VAL
1	A	683	ILE
1	A	684	LEU
1	A	735	ILE
1	A	739	ILE
1	A	772	ARG
1	A	777	LYS
1	A	785	SER
1	A	791	THR
1	A	801	LYS
1	A	803	GLU
1	A	805	ARG

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Mol	Chain	Res	Type
1	A	819	LYS
1	A	824	LEU
1	A	833	VAL
1	B	18	VAL
1	B	27	LYS
1	B	36	THR
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	120	VAL
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	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
1	B	446	MET
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	521	GLU
1	B	534	GLU
1	B	550	LEU

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Mol	Chain	Res	Type
1	B	555	VAL
1	B	560	THR
1	B	574	LYS
1	B	583	VAL
1	B	597	LEU
1	B	599	ILE
1	B	608	GLN
1	B	617	ILE
1	B	654	VAL
1	B	669	VAL
1	B	707	THR
1	B	729	LEU
1	B	736	ILE
1	B	740	ILE
1	B	771	VAL
1	B	777	LYS
1	B	791	THR
1	B	801	LYS
1	B	824	LEU
1	B	833	VAL
2	C	49	GLN
2	C	69	LEU
2	C	71	LEU
2	C	73	LEU
2	D	24	GLU
2	D	42	ARG
2	D	48	LYS
2	D	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	61	HIS
1	A	207	ASN
1	A	333	ASN
1	A	342	GLN
1	A	431	ASN
1	A	442	HIS
1	A	488	GLN
1	A	526	GLN
1	A	551	GLN

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Mol	Chain	Res	Type
1	A	608	GLN
1	A	667	ASN
1	A	726	ASN
1	A	779	GLN
1	B	61	HIS
1	B	63	ASN
1	B	333	ASN
1	B	342	GLN
1	B	351	GLN
1	B	376	GLN
1	B	450	ASN
1	B	498	ASN
1	B	672	HIS
1	B	717	GLN
1	B	727	ASN
1	B	812	GLN
1	B	831	GLN
2	C	49	GLN
2	C	62	GLN
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 oligosaccharides 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	C	76	1,2	2,2,2	0.53	0	0,1,1	-	-
4	NEH	D	76	1,2	2,2,2	0.37	0	0,1,1	-	-

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%)	0.29	23 (3%) 48 39	29, 72, 107, 152	3 (0%)
1	B	681/854 (79%)	0.33	50 (7%) 21 15	45, 70, 116, 159	0
2	C	75/75 (100%)	-0.23	0 100 100	49, 65, 84, 92	0
2	D	75/75 (100%)	-0.08	0 100 100	50, 65, 80, 84	0
All	All	1504/1858 (80%)	0.26	73 (4%) 35 27	29, 70, 109, 159	3 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	617	ILE	6.1
1	B	320	LEU	4.6
1	A	698	PRO	4.4
1	B	411	GLY	4.3
1	A	699	PRO	4.3
1	A	319	PRO	4.1
1	B	203	ASP	4.1
1	B	617	ILE	4.0
1	B	632	LEU	4.0
1	A	76	THR	3.8
1	B	684	LEU	3.6
1	B	282	ASP	3.6
1	B	195	CYS	3.4
1	B	705	VAL	3.4
1	B	768	GLY	3.2
1	A	700	PRO	3.1
1	B	76	THR	3.1
1	B	698	ASP	3.0
1	A	683	ILE	3.0
1	B	156	SER	3.0
1	B	207	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	388	GLU	2.9
1	A	634	GLU	2.9
1	B	633	ASP	2.8
1	B	706	THR	2.8
1	A	684	LEU	2.8
1	B	316	PRO	2.8
1	B	317	LEU	2.7
1	A	206	GLU	2.7
1	B	683	ILE	2.6
1	A	816	ALA	2.6
1	B	518	ALA	2.6
1	A	387	GLY	2.6
1	B	226	GLY	2.6
1	A	223	TYR	2.6
1	B	223	TYR	2.6
1	A	283	MET	2.6
1	B	729	LEU	2.6
1	B	668	TRP	2.5
1	B	4	LEU	2.5
1	B	515	GLU	2.4
1	B	117	ASP	2.4
1	B	228	GLY	2.4
1	B	221	ARG	2.4
1	B	209	TRP	2.4
1	B	749	MET	2.3
1	B	41	GLY	2.3
1	B	388	GLU	2.3
1	A	648	ASP	2.3
1	B	699	PRO	2.3
1	B	700	PRO	2.3
1	A	192	ILE	2.2
1	B	205	ARG	2.2
1	A	195	CYS	2.2
1	B	197	TRP	2.2
1	B	17	ARG	2.2
1	B	194	PRO	2.2
1	B	517	MET	2.2
1	B	283	MET	2.2
1	A	635	SER	2.2
1	B	387	GLY	2.2
1	B	319	PRO	2.2
1	A	266	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	655	TYR	2.1
1	B	769	PRO	2.1
1	B	28	ASP	2.1
1	B	196	GLY	2.1
1	B	138	GLY	2.1
1	A	749	ASP	2.1
1	A	204	MET	2.0
1	A	156	SER	2.0
1	B	175	GLN	2.0
1	B	40	GLU	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 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(Å ²)	Q<0.9
4	NEH	D	76	3/3	0.91	0.16	37,37,37,37	0
5	CL	D	77	1/1	0.93	0.24	84,84,84,84	0
3	ZN	B	836	1/1	0.96	0.06	94,94,94,94	0
4	NEH	C	76	3/3	0.97	0.13	36,36,38,39	0
3	ZN	A	836	1/1	0.99	0.02	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.