



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 11:37 PM UTC

PDB ID : 1Z5S / pdb_00001z5s
Title : Crystal structure of a complex between UBC9, SUMO-1, RANGAP1 and NUP358/RANBP2
Authors : Reverter, D.; Lima, C.D.
Deposited on : 2005-03-19
Resolution : 3.01 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

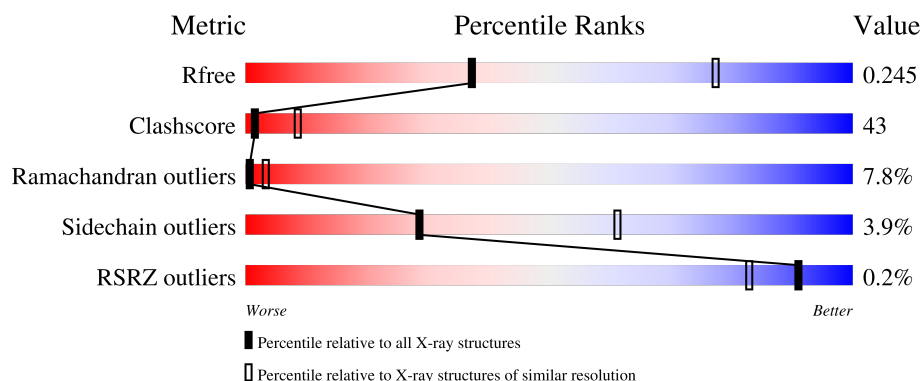
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	158	42% 52% ..
2	B	82	% 30% 57% 7% 5%
3	C	172	30% 52% 8% 9%
4	D	83	17% 58% .. 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3592 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-conjugating enzyme E2 I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1243	800	214	222	7			

- Molecule 2 is a protein called Ubiquitin-like protein SMT3C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			632	398	109	121	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	cloning artifact	UNP P63165
B	17	GLY	-	cloning artifact	UNP P63165

- Molecule 3 is a protein called Ran GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1192	766	196	224	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	416	SER	-	cloning artifact	UNP P46060
C	417	LEU	-	cloning artifact	UNP P46060

- Molecule 4 is a protein called Ran-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	65	Total	C	N	O	S	0	0	0
			497	322	73	101	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2629	SER	-	cloning artifact	UNP P49792
D	2630	LEU	-	cloning artifact	UNP P49792

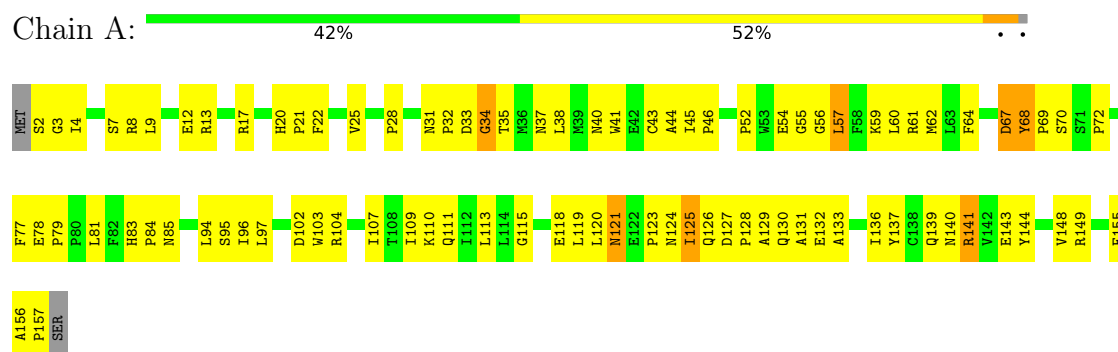
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	4	Total 4	O 4	0	0
5	C	8	Total 8	O 8	0	0
5	D	9	Total 9	O 9	0	0

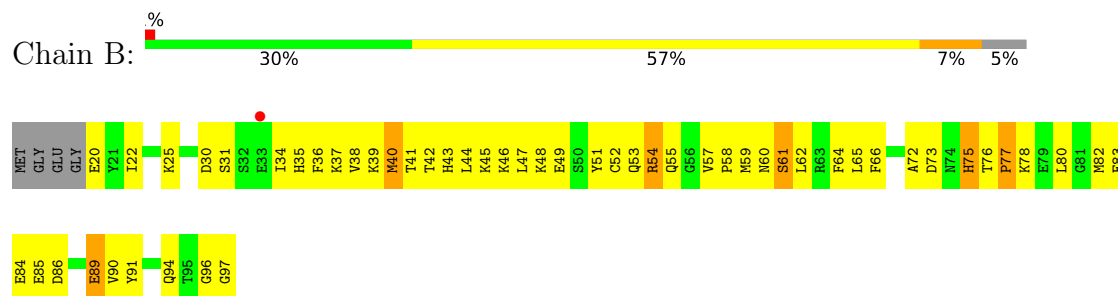
3 Residue-property plots

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.

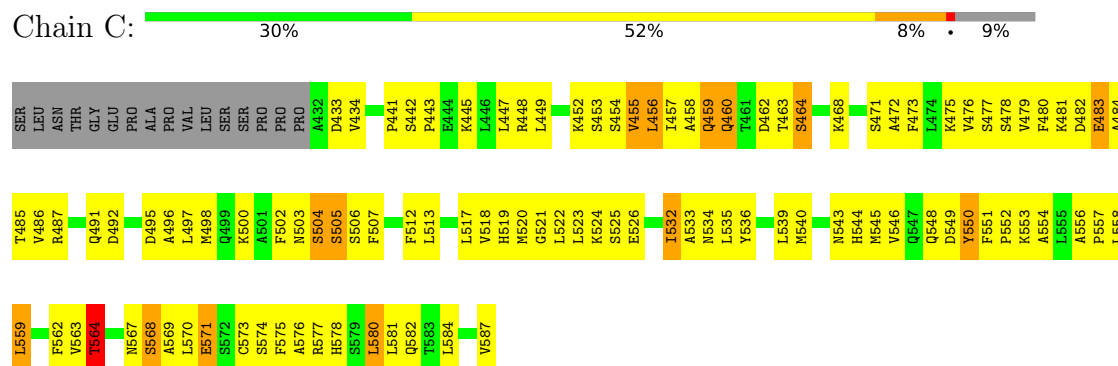
• Molecule 1: Ubiquitin-conjugating enzyme E2 I



• Molecule 2: Ubiquitin-like protein SMT3C

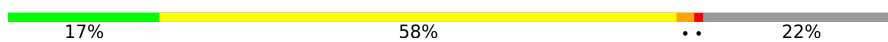


• Molecule 3: Ran GTPase-activating protein 1



• Molecule 4: Ran-binding protein 2

Chain D:



S2693	S2629
GLU	D2630
LYS	D2631
CYS	V2632
ARG	L2633
PRO	L2634
LEU	V2635
GLU	Y2636
GLU	E2637
ASN	L2638
THR	T2639
ALA	P2640
ASP	T2641
GLU	A2642
GLU	E2643
LYS	K2644
GLU	K2645
CYS	L2646
ILE	L2647
	L2651
	K2652
	L2653
	P2654
	P2655
	T2656
	F2657
	F2658
	C2659
	Y2660
	K2661
	N2662
	R2663
	P2664
	D2665
	Y2666
	V2667
	S2668
	E2669
	E2670
	E2671
	E2672
	D2673
	D2674
	E2675
	D2676
	F2677
	V2681
	K2682
	K2683
	L2684
	K2685
	G2686
	K2687
	L2688
	Y2689
	L2690
	D2691

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.12Å 157.12Å 59.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.69 – 3.01 29.69 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.69-3.01) 96.7 (29.69-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.290 0.246 , 0.245	Depositor DCC
R_{free} test set	832 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3592	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/1280	0.93	3/1739 (0.2%)
2	B	0.31	0/642	0.86	1/858 (0.1%)
3	C	0.36	0/1215	0.92	2/1649 (0.1%)
4	D	0.38	0/506	0.91	0/688
All	All	0.39	0/3643	0.91	6/4934 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ASP	N-CA-C	6.89	118.79	111.28
1	A	34	GLY	N-CA-C	-5.97	107.97	115.08
2	B	54	ARG	N-CA-C	-5.66	106.70	113.21
3	C	564	THR	N-CA-C	-5.23	106.40	112.89
1	A	133	ALA	N-CA-C	5.19	117.02	111.36
3	C	571	GLU	N-CA-C	-5.10	107.72	114.04

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	1243	0	1227	92	0
2	B	632	0	628	73	0
3	C	1192	0	1206	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	497	0	475	53	0
5	A	7	0	0	0	0
5	B	4	0	0	0	0
5	C	8	0	0	1	0
5	D	9	0	0	1	0
All	All	3592	0	3536	306	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 43.

All (306) 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)
3:C:534:ASN:HD21	3:C:536:TYR:HB3	1.25	0.99
4:D:2641:THR:HB	4:D:2644:GLN:HG3	1.48	0.95
2:B:38:VAL:HG13	4:D:2632:VAL:HG22	1.57	0.86
3:C:498:MET:HG3	3:C:545:MET:HE2	1.59	0.85
2:B:46:LYS:HE3	4:D:2630:LEU:HD12	1.56	0.84
3:C:546:VAL:HG12	3:C:587:VAL:HG11	1.59	0.83
2:B:58:PRO:HG2	2:B:61:SER:HB2	1.59	0.82
2:B:77:PRO:HG3	2:B:82:MET:HE3	1.61	0.81
1:A:59:LYS:HE2	4:D:2677:PHE:CE2	2.16	0.80
1:A:140:ASN:HD22	1:A:143:GLU:HB2	1.44	0.80
1:A:157:PRO:HG2	4:D:2688:LEU:HD21	1.62	0.80
3:C:563:VAL:HA	3:C:570:LEU:HD21	1.63	0.80
4:D:2684:LEU:C	4:D:2685:ASN:HD22	1.89	0.80
4:D:2685:ASN:ND2	4:D:2686:GLY:H	1.80	0.80
3:C:452:LYS:O	3:C:456:LEU:HB2	1.83	0.79
1:A:129:ALA:HB2	3:C:524:LYS:HE3	1.67	0.77
2:B:36:PHE:HE1	4:D:2634:ILE:HG12	1.48	0.77
4:D:2641:THR:HG22	4:D:2643:GLU:H	1.49	0.75
1:A:125:ILE:HG21	1:A:137:TYR:CD2	2.22	0.73
1:A:4:ILE:HG22	1:A:7:SER:HB2	1.71	0.72
4:D:2658:PHE:HB3	4:D:2661:LYS:HE2	1.71	0.72
3:C:539:LEU:HD23	3:C:580:LEU:HD12	1.72	0.72
1:A:44:ALA:HB1	1:A:57:LEU:HD22	1.71	0.72
2:B:20:GLU:O	2:B:39:LYS:HA	1.91	0.71
3:C:483:GLU:CD	3:C:484:ALA:H	1.99	0.69
3:C:539:LEU:HD11	3:C:570:LEU:HD12	1.72	0.69
2:B:52:CYS:HB3	2:B:57:VAL:O	1.93	0.68
1:A:52:PRO:HB3	1:A:149:ARG:CZ	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:LYS:HG2	2:B:35:HIS:CD2	2.29	0.68
3:C:546:VAL:HG11	3:C:584:LEU:HD23	1.75	0.67
3:C:569:ALA:C	3:C:571:GLU:H	2.01	0.67
2:B:36:PHE:CE1	4:D:2634:ILE:HG12	2.29	0.67
3:C:447:LEU:HD11	3:C:486:VAL:HG22	1.77	0.67
3:C:463:THR:HG21	3:C:500:LYS:HE2	1.76	0.66
3:C:518:VAL:CG1	3:C:525:SER:HB3	2.25	0.66
1:A:125:ILE:HD12	1:A:126:GLN:N	2.10	0.66
2:B:39:LYS:HE3	4:D:2631:ASP:HB2	1.78	0.66
3:C:449:LEU:HB2	3:C:453:SER:HB3	1.77	0.66
2:B:31:SER:HB3	4:D:2656:THR:O	1.96	0.65
3:C:498:MET:HE3	3:C:502:PHE:CE2	2.31	0.65
1:A:85:ASN:HD21	1:A:124:ASN:HB3	1.61	0.65
1:A:94:LEU:HD22	1:A:96:ILE:HB	1.78	0.64
4:D:2641:THR:HG22	4:D:2643:GLU:N	2.12	0.64
1:A:59:LYS:HE2	4:D:2677:PHE:HE2	1.61	0.64
1:A:68:TYR:CD1	1:A:69:PRO:HA	2.33	0.64
3:C:453:SER:C	3:C:455:VAL:H	2.06	0.63
3:C:518:VAL:HG13	3:C:525:SER:HB3	1.80	0.63
3:C:483:GLU:CD	3:C:484:ALA:N	2.56	0.63
2:B:25:LYS:HG2	2:B:35:HIS:NE2	2.14	0.63
1:A:37:ASN:HD22	1:A:38:LEU:N	1.95	0.63
4:D:2661:LYS:O	4:D:2667:VAL:HG21	1.98	0.63
4:D:2641:THR:HB	4:D:2644:GLN:CG	2.26	0.63
2:B:38:VAL:HG22	4:D:2632:VAL:HG13	1.81	0.62
1:A:59:LYS:HG2	1:A:60:LEU:N	2.14	0.62
4:D:2670:GLU:O	4:D:2671:GLU:HG2	2.00	0.61
1:A:144:TYR:O	1:A:148:VAL:HG23	2.00	0.61
3:C:567:ASN:ND2	3:C:570:LEU:H	1.99	0.61
3:C:434:VAL:HG12	3:C:457:ILE:HG12	1.82	0.61
1:A:28:PRO:HA	1:A:41:TRP:HA	1.83	0.60
3:C:559:LEU:O	3:C:563:VAL:HG23	2.01	0.60
1:A:141:ARG:HG2	1:A:141:ARG:NH2	2.17	0.60
2:B:80:LEU:HD12	2:B:82:MET:HE2	1.83	0.60
3:C:534:ASN:HD21	3:C:536:TYR:CB	2.07	0.60
1:A:31:ASN:HB3	1:A:32:PRO:HD2	1.83	0.60
1:A:121:ASN:C	1:A:123:PRO:HD3	2.27	0.60
3:C:584:LEU:HA	3:C:587:VAL:HG22	1.84	0.59
1:A:2:SER:CA	1:A:67:ASP:HA	2.33	0.59
3:C:568:SER:O	3:C:571:GLU:HB2	2.02	0.59
3:C:552:PRO:C	3:C:554:ALA:H	2.08	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:CD2	1:A:96:ILE:HB	2.32	0.59
1:A:140:ASN:HD22	1:A:143:GLU:CB	2.15	0.59
1:A:54:GLU:HG2	1:A:55:GLY:N	2.18	0.58
1:A:141:ARG:HG2	1:A:141:ARG:HH21	1.66	0.58
3:C:504:SER:O	3:C:506:SER:N	2.36	0.58
2:B:72:ALA:H	2:B:75:HIS:HD2	1.52	0.58
3:C:549:ASP:C	3:C:551:PHE:H	2.10	0.58
2:B:39:LYS:HB2	2:B:42:THR:HG23	1.85	0.58
4:D:2660:TYR:CE1	4:D:2661:LYS:HB3	2.39	0.58
3:C:564:THR:HA	3:C:577:ARG:HH21	1.68	0.58
1:A:37:ASN:HD22	1:A:37:ASN:C	2.10	0.57
1:A:137:TYR:OH	1:A:141:ARG:NH1	2.35	0.57
3:C:580:LEU:HD22	3:C:584:LEU:CD1	2.34	0.57
4:D:2684:LEU:C	4:D:2685:ASN:ND2	2.61	0.57
1:A:94:LEU:HD23	1:A:96:ILE:H	1.68	0.57
2:B:35:HIS:HB2	4:D:2636:TYR:HB3	1.86	0.57
3:C:442:SER:HB3	3:C:445:LYS:HB2	1.85	0.56
3:C:563:VAL:CA	3:C:570:LEU:HD21	2.35	0.56
1:A:85:ASN:HD22	2:B:97:GLY:H	1.52	0.56
2:B:75:HIS:CE1	2:B:80:LEU:HG	2.41	0.56
1:A:115:GLY:O	1:A:118:GLU:HG2	2.07	0.55
2:B:76:THR:C	2:B:78:LYS:N	2.64	0.55
4:D:2690:LEU:HD12	4:D:2691:ASP:N	2.21	0.55
3:C:479:VAL:C	3:C:481:LYS:HE2	2.32	0.55
3:C:481:LYS:C	3:C:483:GLU:H	2.12	0.55
4:D:2685:ASN:ND2	4:D:2686:GLY:N	2.54	0.55
1:A:140:ASN:ND2	1:A:143:GLU:H	2.05	0.55
2:B:49:GLU:HG2	2:B:59:MET:CE	2.37	0.55
2:B:37:LYS:HG3	4:D:2635:VAL:HG21	1.89	0.54
2:B:45:LYS:HB2	2:B:73:ASP:O	2.07	0.54
2:B:76:THR:C	2:B:78:LYS:H	2.15	0.54
1:A:96:ILE:HD12	2:B:94:GLN:OE1	2.07	0.54
1:A:107:ILE:HA	1:A:111:GLN:OE1	2.07	0.54
3:C:462:ASP:HB3	3:C:468:LYS:HD3	1.89	0.54
3:C:534:ASN:CG	3:C:536:TYR:H	2.16	0.54
2:B:54:ARG:HG2	4:D:2634:ILE:HD13	1.90	0.54
3:C:498:MET:HE1	3:C:512:PHE:CE2	2.43	0.54
1:A:125:ILE:C	1:A:127:ASP:H	2.15	0.54
2:B:54:ARG:HG3	2:B:54:ARG:O	2.07	0.54
3:C:434:VAL:CG1	3:C:456:LEU:HD22	2.38	0.54
3:C:453:SER:C	3:C:455:VAL:N	2.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:LYS:O	2:B:49:GLU:HG3	2.08	0.53
4:D:2653:LEU:HD13	4:D:2657:PHE:CD2	2.43	0.53
3:C:569:ALA:C	3:C:571:GLU:N	2.65	0.53
1:A:52:PRO:HA	1:A:149:ARG:NH1	2.23	0.53
2:B:20:GLU:N	2:B:40:MET:HE3	2.22	0.53
1:A:140:ASN:ND2	1:A:143:GLU:HB2	2.19	0.53
2:B:47:LEU:C	2:B:47:LEU:HD23	2.34	0.53
3:C:480:PHE:C	3:C:480:PHE:CD2	2.87	0.53
3:C:567:ASN:HD22	3:C:570:LEU:HB2	1.74	0.53
3:C:570:LEU:O	3:C:577:ARG:HD2	2.08	0.53
2:B:25:LYS:HE2	2:B:35:HIS:NE2	2.24	0.52
3:C:471:SER:O	3:C:475:LYS:HG3	2.09	0.52
1:A:44:ALA:HB1	1:A:57:LEU:CD2	2.39	0.52
3:C:575:PHE:HB3	5:C:5:HOH:O	2.08	0.52
2:B:44:LEU:HD12	2:B:75:HIS:HB3	1.92	0.52
3:C:495:ASP:HA	3:C:550:TYR:OH	2.10	0.51
3:C:520:MET:O	3:C:522:LEU:HG	2.09	0.51
2:B:76:THR:O	2:B:78:LYS:N	2.43	0.51
2:B:89:GLU:HB3	2:B:91:TYR:CE1	2.45	0.51
1:A:118:GLU:HG3	1:A:119:LEU:N	2.26	0.51
3:C:567:ASN:HD22	3:C:570:LEU:CB	2.23	0.51
1:A:62:MET:HE1	1:A:113:LEU:HD21	1.91	0.51
2:B:60:ASN:O	2:B:62:LEU:N	2.42	0.51
4:D:2641:THR:HG22	4:D:2642:ALA:N	2.24	0.51
3:C:476:VAL:O	3:C:479:VAL:HG22	2.11	0.51
4:D:2641:THR:CG2	4:D:2642:ALA:N	2.74	0.51
1:A:94:LEU:HD11	2:B:94:GLN:NE2	2.26	0.51
3:C:544:HIS:CE1	3:C:548:GLN:NE2	2.79	0.51
1:A:68:TYR:CG	1:A:69:PRO:HA	2.47	0.50
2:B:25:LYS:HE2	2:B:35:HIS:CE1	2.47	0.50
3:C:472:ALA:HB3	3:C:497:LEU:HD21	1.94	0.50
3:C:532:ILE:N	3:C:532:ILE:HD13	2.27	0.50
4:D:2685:ASN:HD22	4:D:2686:GLY:H	1.54	0.50
4:D:2685:ASN:HD22	4:D:2686:GLY:N	2.10	0.50
4:D:2663:ARG:HB3	4:D:2664:PRO:HD2	1.94	0.50
1:A:40:ASN:HD21	1:A:61:ARG:HD3	1.77	0.49
2:B:34:ILE:HD12	2:B:51:TYR:CE1	2.47	0.49
2:B:39:LYS:C	2:B:41:THR:H	2.20	0.49
4:D:2682:LYS:O	4:D:2685:ASN:N	2.43	0.49
4:D:2651:LEU:C	4:D:2652:LYS:HG2	2.37	0.49
4:D:2676:ASP:O	4:D:2677:PHE:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:O	1:A:43:CYS:HA	2.12	0.49
3:C:549:ASP:C	3:C:551:PHE:N	2.70	0.49
4:D:2653:LEU:HB3	4:D:2654:PRO:HD2	1.93	0.49
1:A:119:LEU:HD12	1:A:119:LEU:O	2.13	0.49
3:C:481:LYS:C	3:C:483:GLU:N	2.69	0.49
3:C:518:VAL:HG11	3:C:525:SER:HB3	1.95	0.49
3:C:567:ASN:O	3:C:571:GLU:HG3	2.12	0.49
1:A:85:ASN:HD22	2:B:97:GLY:N	2.11	0.49
1:A:32:PRO:C	1:A:34:GLY:H	2.21	0.49
3:C:536:TYR:CD1	3:C:576:ALA:HB2	2.48	0.49
1:A:12:GLU:OE2	1:A:109:ILE:HG13	2.12	0.48
3:C:477:SER:C	3:C:479:VAL:H	2.20	0.48
3:C:540:MET:O	3:C:543:ASN:HB3	2.12	0.48
2:B:48:LYS:HG3	2:B:64:PHE:CE1	2.48	0.48
4:D:2690:LEU:HD12	4:D:2690:LEU:C	2.38	0.48
3:C:443:PRO:CG	3:C:481:LYS:HE3	2.42	0.48
3:C:457:ILE:C	3:C:459:GLN:H	2.21	0.48
3:C:571:GLU:C	3:C:573:CYS:H	2.22	0.48
3:C:473:PHE:CD1	3:C:473:PHE:C	2.91	0.48
1:A:67:ASP:O	1:A:68:TYR:C	2.56	0.48
1:A:128:PRO:O	3:C:524:LYS:HG2	2.14	0.48
3:C:552:PRO:C	3:C:554:ALA:N	2.71	0.48
3:C:556:ALA:HB3	3:C:557:PRO:CD	2.43	0.48
1:A:83:HIS:CE1	1:A:85:ASN:H	2.31	0.48
1:A:94:LEU:HB3	1:A:97:LEU:HD12	1.94	0.48
1:A:130:GLN:O	1:A:130:GLN:HG3	2.13	0.48
1:A:8:ARG:NH1	4:D:2651:LEU:O	2.45	0.47
2:B:62:LEU:HD13	2:B:90:VAL:HG11	1.96	0.47
2:B:57:VAL:HG11	2:B:62:LEU:HD21	1.96	0.47
3:C:481:LYS:O	3:C:483:GLU:N	2.48	0.47
3:C:558:LEU:N	3:C:558:LEU:HD12	2.30	0.47
1:A:45:ILE:HG22	1:A:46:PRO:O	2.14	0.47
3:C:584:LEU:O	3:C:587:VAL:HG22	2.14	0.47
1:A:37:ASN:C	1:A:37:ASN:ND2	2.73	0.47
3:C:447:LEU:C	3:C:449:LEU:H	2.22	0.47
3:C:483:GLU:OE1	3:C:485:THR:N	2.47	0.47
2:B:53:GLN:C	2:B:55:GLN:H	2.23	0.47
3:C:462:ASP:OD1	3:C:464:SER:HB2	2.15	0.47
1:A:13:ARG:O	1:A:17:ARG:HG3	2.15	0.47
1:A:61:ARG:NE	1:A:78:GLU:OE2	2.48	0.47
1:A:104:ARG:HE	1:A:104:ARG:HB2	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:PRO:HB2	2:B:60:ASN:OD1	2.15	0.47
3:C:536:TYR:HD1	3:C:576:ALA:HB2	1.80	0.47
1:A:121:ASN:O	1:A:123:PRO:HD3	2.15	0.46
2:B:89:GLU:HB3	2:B:91:TYR:HE1	1.78	0.46
3:C:546:VAL:CG1	3:C:587:VAL:HG11	2.37	0.46
3:C:453:SER:O	3:C:455:VAL:N	2.48	0.46
2:B:64:PHE:CD1	2:B:64:PHE:N	2.83	0.46
1:A:79:PRO:HD2	1:A:155:PHE:HE2	1.80	0.46
2:B:60:ASN:O	2:B:61:SER:C	2.59	0.46
4:D:2684:LEU:O	4:D:2686:GLY:N	2.49	0.46
2:B:44:LEU:HD11	2:B:82:MET:HE1	1.98	0.46
3:C:505:SER:C	3:C:507:PHE:H	2.24	0.46
1:A:125:ILE:HD12	1:A:126:GLN:H	1.77	0.46
3:C:487:ARG:O	3:C:491:GLN:HG3	2.15	0.46
1:A:77:PHE:CE1	1:A:81:LEU:HD12	2.51	0.46
2:B:66:PHE:CZ	2:B:82:MET:HG2	2.52	0.45
2:B:42:THR:HG22	4:D:2630:LEU:HD22	1.97	0.45
4:D:2660:TYR:HA	5:D:11:HOH:O	2.16	0.45
1:A:148:VAL:O	1:A:149:ARG:C	2.60	0.45
2:B:43:HIS:HA	2:B:76:THR:OG1	2.16	0.45
3:C:580:LEU:CD2	3:C:584:LEU:HG	2.46	0.45
2:B:85:GLU:O	2:B:85:GLU:HG3	2.17	0.45
3:C:443:PRO:HA	3:C:479:VAL:HB	1.99	0.45
4:D:2685:ASN:HD22	4:D:2685:ASN:N	2.12	0.45
1:A:94:LEU:HD23	1:A:94:LEU:C	2.42	0.45
2:B:48:LYS:HE2	2:B:59:MET:HG3	1.99	0.45
3:C:534:ASN:ND2	3:C:536:TYR:HB3	2.10	0.45
4:D:2647:LEU:HD23	4:D:2658:PHE:CE1	2.51	0.45
1:A:9:LEU:HD21	1:A:64:PHE:CD2	2.52	0.45
2:B:54:ARG:O	2:B:54:ARG:CG	2.63	0.45
2:B:76:THR:HG23	2:B:77:PRO:HD2	1.99	0.44
3:C:519:HIS:O	3:C:532:ILE:HD12	2.16	0.44
4:D:2674:ASP:O	4:D:2675:GLU:C	2.59	0.44
4:D:2659:CYS:HA	4:D:2662:ASN:HB2	1.99	0.44
3:C:434:VAL:HG13	3:C:456:LEU:HD22	1.99	0.44
3:C:587:VAL:HG23	3:C:587:VAL:OXT	2.18	0.44
1:A:72:PRO:HB3	1:A:103:TRP:CD2	2.52	0.44
1:A:21:PRO:HD3	1:A:110:LYS:HG3	2.00	0.44
3:C:487:ARG:HG3	3:C:491:GLN:HE21	1.83	0.44
3:C:552:PRO:O	3:C:554:ALA:N	2.50	0.44
1:A:56:GLY:HA2	1:A:156:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:480:PHE:CE1	3:C:487:ARG:HB2	2.53	0.44
3:C:532:ILE:H	3:C:532:ILE:CD1	2.31	0.44
3:C:535:LEU:O	3:C:539:LEU:HB2	2.18	0.44
3:C:433:ASP:HB3	3:C:449:LEU:CD2	2.48	0.44
1:A:83:HIS:O	1:A:130:GLN:NE2	2.50	0.43
2:B:22:ILE:HG13	2:B:22:ILE:O	2.18	0.43
1:A:32:PRO:C	1:A:34:GLY:N	2.76	0.43
3:C:546:VAL:HG11	3:C:584:LEU:CD2	2.46	0.43
3:C:563:VAL:O	3:C:570:LEU:HD21	2.18	0.43
1:A:85:ASN:ND2	2:B:96:GLY:HA3	2.34	0.43
2:B:76:THR:HG22	2:B:78:LYS:H	1.84	0.43
3:C:479:VAL:O	3:C:481:LYS:HE2	2.19	0.43
2:B:57:VAL:HG12	2:B:61:SER:HB3	2.00	0.43
2:B:65:LEU:HD12	2:B:91:TYR:CE1	2.53	0.43
4:D:2681:VAL:O	4:D:2684:LEU:HB3	2.18	0.43
1:A:85:ASN:ND2	1:A:124:ASN:HB3	2.31	0.43
2:B:49:GLU:HG2	2:B:59:MET:HE1	1.99	0.43
1:A:69:PRO:O	1:A:70:SER:C	2.62	0.43
1:A:4:ILE:HG22	1:A:4:ILE:O	2.19	0.42
3:C:503:ASN:O	3:C:504:SER:HB3	2.19	0.42
4:D:2638:LEU:HD23	4:D:2639:THR:N	2.34	0.42
3:C:549:ASP:O	3:C:551:PHE:N	2.52	0.42
3:C:582:GLN:NE2	3:C:582:GLN:HA	2.34	0.42
2:B:57:VAL:CG1	2:B:61:SER:HB3	2.49	0.42
2:B:80:LEU:CB	2:B:82:MET:HG3	2.49	0.42
3:C:504:SER:C	3:C:506:SER:N	2.77	0.42
3:C:564:THR:HG23	3:C:581:LEU:CD2	2.50	0.42
2:B:66:PHE:CE2	2:B:82:MET:HG2	2.55	0.42
1:A:8:ARG:HD3	1:A:68:TYR:CE2	2.54	0.42
1:A:77:PHE:CD1	1:A:81:LEU:HD12	2.55	0.42
3:C:523:LEU:HD12	3:C:524:LYS:H	1.85	0.42
1:A:95:SER:HB2	1:A:102:ASP:OD1	2.19	0.42
1:A:136:ILE:HD13	1:A:139:GLN:NE2	2.35	0.42
3:C:577:ARG:O	3:C:578:HIS:C	2.62	0.42
3:C:517:LEU:HD13	3:C:562:PHE:CG	2.55	0.42
1:A:62:MET:HG2	1:A:64:PHE:CE1	2.55	0.41
2:B:38:VAL:HG12	2:B:39:LYS:N	2.35	0.41
3:C:459:GLN:HA	3:C:500:LYS:NZ	2.35	0.41
3:C:492:ASP:HA	3:C:495:ASP:HB2	2.02	0.41
3:C:551:PHE:HA	3:C:552:PRO:HD3	1.92	0.41
1:A:83:HIS:H	1:A:130:GLN:NE2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ALA:O	1:A:132:GLU:C	2.63	0.41
3:C:496:ALA:O	3:C:497:LEU:C	2.62	0.41
3:C:556:ALA:HB3	3:C:557:PRO:HD3	2.00	0.41
1:A:62:MET:HE1	1:A:113:LEU:CD2	2.50	0.41
1:A:94:LEU:HD12	1:A:119:LEU:CD2	2.50	0.41
1:A:83:HIS:H	1:A:130:GLN:HE22	1.67	0.41
2:B:39:LYS:CE	4:D:2631:ASP:HB2	2.46	0.41
2:B:25:LYS:HE2	2:B:35:HIS:HE2	1.85	0.41
2:B:60:ASN:CG	2:B:61:SER:N	2.78	0.41
3:C:460:GLN:O	3:C:460:GLN:NE2	2.53	0.41
2:B:41:THR:O	2:B:41:THR:HG22	2.21	0.41
2:B:49:GLU:HA	2:B:59:MET:HE1	2.03	0.41
3:C:558:LEU:N	3:C:558:LEU:CD1	2.83	0.41
4:D:2637:GLU:HG3	4:D:2637:GLU:O	2.20	0.41
4:D:2647:LEU:CD2	4:D:2658:PHE:CZ	3.03	0.41
1:A:140:ASN:ND2	1:A:143:GLU:N	2.69	0.41
3:C:477:SER:O	3:C:479:VAL:N	2.54	0.41
3:C:513:LEU:C	3:C:513:LEU:HD13	2.46	0.41
1:A:17:ARG:HD3	4:D:2673:ASP:OD2	2.21	0.40
1:A:22:PHE:CD2	4:D:2690:LEU:HB3	2.57	0.40
1:A:61:ARG:HB2	1:A:78:GLU:OE2	2.20	0.40
1:A:119:LEU:O	1:A:120:LEU:C	2.63	0.40
3:C:520:MET:HA	3:C:532:ILE:CD1	2.51	0.40
4:D:2640:PRO:HG2	4:D:2645:LYS:HB2	2.03	0.40
2:B:22:ILE:HG22	2:B:84:GLU:HG3	2.02	0.40
1:A:20:HIS:HB2	1:A:21:PRO:HD2	2.04	0.40
1:A:54:GLU:CG	1:A:55:GLY:N	2.84	0.40
1:A:94:LEU:HD12	1:A:119:LEU:HD22	2.03	0.40
3:C:526:GLU:O	3:C:526:GLU:HG2	2.21	0.40
3:C:534:ASN:OD1	3:C:536:TYR:N	2.52	0.40
2:B:45:LYS:HD2	2:B:73:ASP:OD2	2.21	0.40
3:C:573:CYS:O	3:C:574:SER:C	2.63	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	154/158 (98%)	124 (80%)	26 (17%)	4 (3%)	4	21
2	B	76/82 (93%)	59 (78%)	11 (14%)	6 (8%)	1	3
3	C	154/172 (90%)	104 (68%)	33 (21%)	17 (11%)	0	1
4	D	63/83 (76%)	44 (70%)	11 (18%)	8 (13%)	0	1
All	All	447/495 (90%)	331 (74%)	81 (18%)	35 (8%)	1	3

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	THR
2	B	61	SER
3	C	504	SER
3	C	505	SER
4	D	2665	ASP
4	D	2685	ASN
3	C	478	SER
3	C	483	GLU
3	C	533	ALA
3	C	553	LYS
4	D	2687	LYS
1	A	3	GLY
1	A	33	ASP
2	B	40	MET
2	B	86	ASP
3	C	441	PRO
3	C	454	SER
3	C	464	SER
3	C	482	ASP
3	C	550	TYR
4	D	2666	TYR
4	D	2668	SER
4	D	2669	GLU
2	B	83	GLU
3	C	448	ARG
3	C	459	GLN
4	D	2686	GLY
2	B	30	ASP

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Mol	Chain	Res	Type
3	C	568	SER
3	C	458	ALA
4	D	2655	PRO
1	A	68	TYR
2	B	77	PRO
3	C	521	GLY
3	C	455	VAL

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	132/137 (96%)	127 (96%)	5 (4%)	29	62
2	B	70/73 (96%)	68 (97%)	2 (3%)	37	68
3	C	133/150 (89%)	127 (96%)	6 (4%)	24	57
4	D	52/76 (68%)	50 (96%)	2 (4%)	29	62
All	All	387/436 (89%)	372 (96%)	15 (4%)	28	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	84	PRO
1	A	121	ASN
1	A	125	ILE
1	A	141	ARG
2	B	75	HIS
2	B	89	GLU
3	C	456	LEU
3	C	460	GLN
3	C	532	ILE
3	C	559	LEU
3	C	564	THR
3	C	580	LEU
4	D	2655	PRO

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Mol	Chain	Res	Type
4	D	2685	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	121	ASN
1	A	139	GLN
1	A	140	ASN
2	B	43	HIS
2	B	74	ASN
2	B	75	HIS
3	C	460	GLN
3	C	499	GLN
3	C	503	ASN
3	C	544	HIS
3	C	548	GLN
3	C	567	ASN
3	C	578	HIS
3	C	582	GLN
4	D	2685	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	156/158 (98%)	-0.30	0 100 100	47, 73, 92, 98	0
2	B	78/82 (95%)	0.14	1 (1%) 75 53	69, 111, 144, 157	0
3	C	156/172 (90%)	-0.20	0 100 100	63, 91, 115, 122	0
4	D	65/83 (78%)	0.03	0 100 100	56, 97, 143, 149	0
All	All	455/495 (91%)	-0.14	1 (0%) 91 83	47, 86, 137, 157	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	GLU	2.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.