



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 AM UTC

PDB ID : 5KYU / pdb_00005kyu
Title : crystal structure of Sec23 and TANGO1 peptide2 complex
Authors : Ma, W.; Goldberg, J.
Deposited on : 2016-07-22
Resolution : 3.51 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

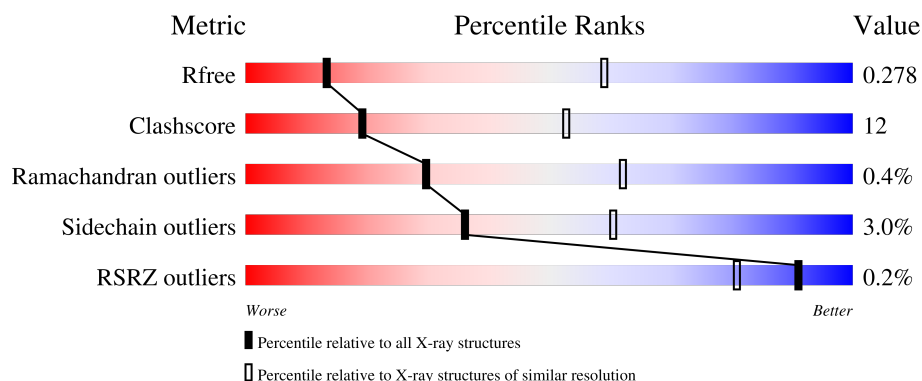
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	765	 75% 18% 6%
2	B	767	 73% 23%
3	C	8	 25% 12% 62%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	B	1101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11605 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	716	Total	C	N	O	S	0	0	0
			5678	3617	975	1046	40			

- Molecule 2 is a protein called Protein transport protein Sec24D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	764	Total	C	N	O	S	0	0	0
			5904	3758	993	1101	52			

- Molecule 3 is a protein called TANGO1 peptide2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			21	15	3	3			

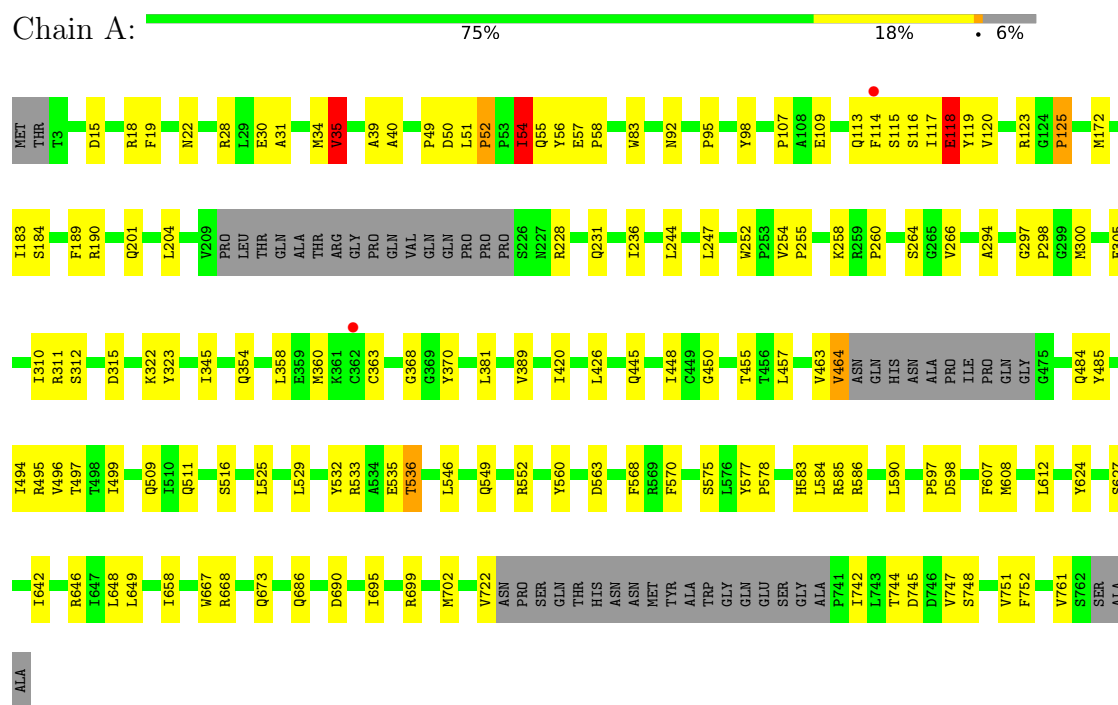
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

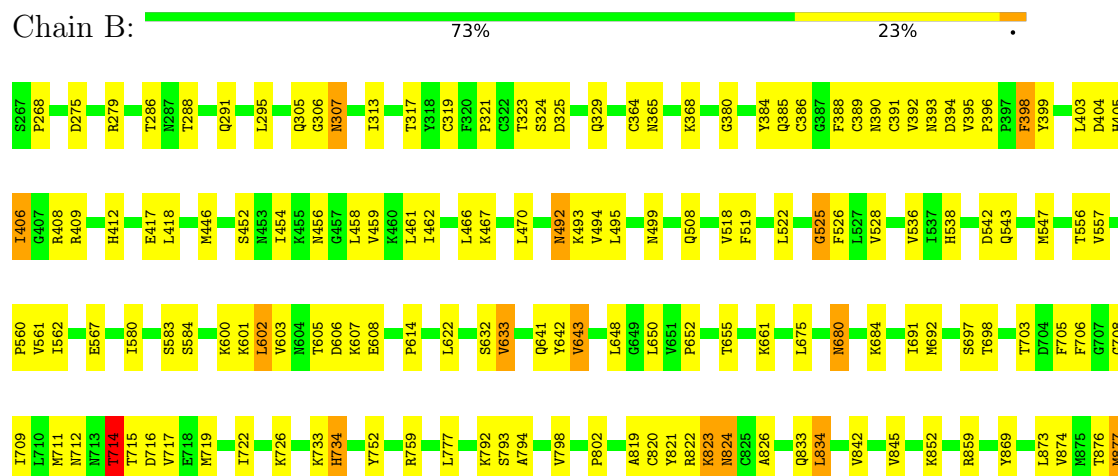
3 Residue-property plots [i](#)

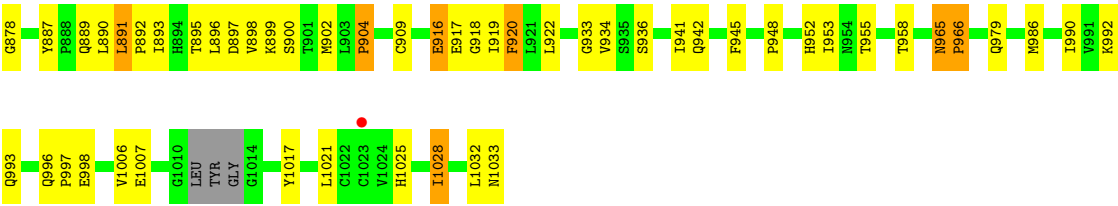
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein transport protein Sec23A

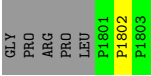


• Molecule 2: Protein transport protein Sec24D





● Molecule 3: TANGO1 peptide2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.43Å 140.93Å 150.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.55 – 3.51 48.55 – 3.51	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.55-3.51) 91.3 (48.55-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.217 , 0.267 0.235 , 0.278	Depositor DCC
R_{free} test set	1998 reflections (7.10%)	wwPDB-VP
Wilson B-factor (Å ²)	112.8	Xtriage
Anisotropy	0.680	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 112.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11605	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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	0.29	1/5811 (0.0%)	0.44	5/7870 (0.1%)
2	B	0.33	1/6029 (0.0%)	0.60	17/8181 (0.2%)
3	C	0.21	0/23	0.39	0/32
All	All	0.31	2/11863 (0.0%)	0.53	22/16083 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	GLU	CA-C	-9.26	1.41	1.52
2	B	395	VAL	C-N	5.19	1.39	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	715	THR	N-CA-C	10.19	122.38	111.28
2	B	824	ASN	N-CA-C	10.02	121.96	111.14
2	B	918	GLY	N-CA-C	9.50	124.39	112.14
2	B	878	GLY	N-CA-C	-8.52	101.06	112.82
2	B	525	GLY	N-CA-C	-8.44	101.12	115.80
2	B	823	LYS	N-CA-C	7.05	118.75	111.14
1	A	54	ILE	N-CA-C	7.02	117.81	110.72
2	B	877	MET	N-CA-C	6.78	120.32	110.28
2	B	395	VAL	CA-C-N	-6.45	113.74	120.38
2	B	395	VAL	C-N-CA	-6.45	113.74	120.38
2	B	716	ASP	N-CA-C	6.36	119.31	109.07
2	B	902	MET	N-CA-C	6.20	118.04	111.28
1	A	52	PRO	CA-C-N	-5.72	113.86	119.76
1	A	52	PRO	C-N-CA	-5.72	113.86	119.76
2	B	712	ASN	N-CA-C	-5.54	105.63	112.72
2	B	394	ASP	N-CA-C	-5.41	101.64	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LEU	CA-C-N	-5.23	115.00	120.38
1	A	51	LEU	C-N-CA	-5.23	115.00	120.38
2	B	916	GLU	CA-C-N	5.17	127.21	120.28
2	B	916	GLU	C-N-CA	5.17	127.21	120.28
2	B	714	THR	N-CA-C	-5.16	105.66	111.28
2	B	715	THR	CB-CA-C	-5.10	102.33	110.79

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	5678	0	5616	105	0
2	B	5904	0	5808	166	0
3	C	21	0	21	1	0
4	A	1	0	0	0	0
4	B	1	0	0	2	0
All	All	11605	0	11445	270	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 12.

All (270) 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:B:385:GLN:HE21	2:B:390:ASN:HB3	1.32	0.93
1:A:15:ASP:OD1	1:A:115:SER:OG	1.90	0.90
2:B:403:LEU:HD12	2:B:404:ASP:H	1.35	0.89
2:B:916:GLU:O	2:B:933:GLY:HA3	1.75	0.87
2:B:389:CYS:HG	4:B:1101:ZN:ZN	0.84	0.86
2:B:874:VAL:HA	2:B:877:MET:HG3	1.58	0.85
1:A:116:SER:HB3	1:A:497:THR:HG23	1.57	0.85
2:B:396:PRO:HB2	2:B:398:PHE:CE1	2.12	0.84
2:B:705:PHE:C	2:B:706:PHE:HD1	1.84	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:PHE:HE2	2:B:793:SER:HA	1.40	0.83
2:B:364:CYS:HA	2:B:393:ASN:ND2	1.93	0.83
2:B:404:ASP:CB	2:B:408:ARG:O	2.26	0.83
2:B:891:LEU:HD12	2:B:904:PRO:HG2	1.62	0.82
2:B:396:PRO:HB2	2:B:398:PHE:HE1	1.47	0.79
2:B:403:LEU:CD1	2:B:404:ASP:H	1.98	0.77
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.66	0.76
1:A:55:GLN:HA	1:A:120:VAL:HB	1.68	0.75
2:B:602:LEU:HD12	2:B:603:VAL:HG23	1.69	0.74
2:B:705:PHE:C	2:B:706:PHE:CD1	2.65	0.74
2:B:389:CYS:SG	4:B:1101:ZN:ZN	1.78	0.73
2:B:275:ASP:HB3	2:B:295:LEU:HD12	1.72	0.71
1:A:563:ASP:H	1:A:761:VAL:HB	1.56	0.71
1:A:54:ILE:HG21	1:A:56:TYR:CZ	2.25	0.70
2:B:412:HIS:CE1	2:B:418:LEU:O	2.44	0.70
2:B:897:ASP:O	2:B:900:SER:OG	2.04	0.70
2:B:889:GLN:HG2	2:B:891:LEU:HD21	1.72	0.70
1:A:499:ILE:C	1:A:499:ILE:HD12	2.17	0.69
1:A:499:ILE:HD12	1:A:499:ILE:O	1.93	0.68
2:B:364:CYS:HA	2:B:393:ASN:HD21	1.58	0.68
2:B:823:LYS:HG3	2:B:824:ASN:ND2	2.09	0.67
1:A:49:PRO:CD	1:A:50:ASP:H	2.07	0.67
2:B:396:PRO:CB	2:B:398:PHE:HE1	2.06	0.67
2:B:492:ASN:O	2:B:492:ASN:ND2	2.22	0.67
2:B:822:ARG:HG2	2:B:1028:ILE:HG23	1.76	0.67
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.77	0.67
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.77	0.67
2:B:633:VAL:H	2:B:655:THR:HG21	1.60	0.67
2:B:708:GLY:C	2:B:709:ILE:HG23	2.20	0.66
1:A:49:PRO:HD2	1:A:50:ASP:H	1.58	0.66
1:A:54:ILE:N	1:A:54:ILE:HD13	2.11	0.66
2:B:403:LEU:HD12	2:B:404:ASP:N	2.10	0.65
2:B:823:LYS:HB2	2:B:1033:ASN:HB3	1.77	0.65
1:A:118:GLU:HG3	1:A:495:ARG:HD3	1.78	0.65
2:B:385:GLN:NE2	2:B:390:ASN:HB3	2.09	0.65
1:A:312:SER:H	1:A:315:ASP:HB2	1.62	0.64
1:A:34:MET:O	1:A:35:VAL:HG12	1.96	0.64
1:A:532:TYR:O	1:A:536:THR:OG1	2.16	0.64
2:B:399:TYR:OH	2:B:417:GLU:OE2	2.14	0.64
1:A:118:GLU:OE2	1:A:485:TYR:OH	2.12	0.64
1:A:533:ARG:HA	1:A:536:THR:OG1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ARG:HG2	2:B:1028:ILE:CG2	2.28	0.64
2:B:385:GLN:HG3	2:B:390:ASN:O	1.98	0.64
2:B:365:ASN:H	2:B:393:ASN:HD21	1.45	0.64
2:B:385:GLN:HE21	2:B:390:ASN:CB	2.09	0.64
1:A:15:ASP:OD2	1:A:499:ILE:HG22	1.98	0.63
2:B:286:THR:OG1	2:B:305:GLN:O	2.15	0.63
1:A:117:ILE:HD11	1:A:119:TYR:OH	1.99	0.62
1:A:31:ALA:HA	1:A:34:MET:CG	2.29	0.62
2:B:891:LEU:N	2:B:891:LEU:HD22	2.14	0.62
2:B:820:CYS:HA	2:B:823:LYS:HG2	1.80	0.62
2:B:706:PHE:HD2	2:B:792:LYS:HB3	1.65	0.61
1:A:667:TRP:CE2	3:C:1802:PRO:HB2	2.34	0.61
2:B:493:LYS:HA	2:B:557:VAL:HG13	1.83	0.61
2:B:386:CYS:O	2:B:390:ASN:HA	2.01	0.60
2:B:819:ALA:HA	2:B:1028:ILE:HG12	1.83	0.60
1:A:368:GLY:HA3	1:A:450:GLY:O	2.01	0.60
2:B:391:CYS:SG	2:B:392:VAL:N	2.75	0.60
2:B:890:LEU:C	2:B:891:LEU:HD22	2.26	0.60
1:A:54:ILE:CG2	1:A:56:TYR:CE2	2.85	0.60
2:B:602:LEU:HD21	2:B:859:ARG:HB2	1.84	0.59
1:A:113:GLN:NE2	1:A:114:PHE:CE2	2.63	0.59
1:A:54:ILE:HG22	1:A:56:TYR:CE2	2.38	0.59
1:A:15:ASP:O	1:A:497:THR:HG21	2.02	0.58
1:A:311:ARG:NH2	1:A:598:ASP:OD1	2.36	0.58
1:A:172:MET:HE2	1:A:252:TRP:HE1	1.68	0.58
2:B:467:LYS:NZ	2:B:542:ASP:OD1	2.29	0.58
1:A:54:ILE:O	1:A:55:GLN:HB2	2.02	0.58
1:A:31:ALA:HA	1:A:34:MET:HG2	1.86	0.57
1:A:624:TYR:HB2	1:A:649:LEU:HB3	1.86	0.57
2:B:823:LYS:HG3	2:B:824:ASN:N	2.18	0.57
2:B:706:PHE:CE2	2:B:793:SER:HA	2.31	0.56
2:B:708:GLY:O	2:B:709:ILE:CG2	2.53	0.56
2:B:600:LYS:HA	2:B:859:ARG:NH1	2.19	0.56
2:B:920:PHE:CD1	2:B:920:PHE:N	2.73	0.56
1:A:30:GLU:O	1:A:34:MET:HG2	2.06	0.56
1:A:204:LEU:O	1:A:228:ARG:NH2	2.39	0.56
2:B:706:PHE:HD1	2:B:706:PHE:N	2.03	0.56
2:B:499:ASN:HB3	2:B:508:GLN:HB2	1.87	0.56
2:B:602:LEU:HA	2:B:608:GLU:HB2	1.87	0.56
1:A:668:ARG:HG2	1:A:673:GLN:HE22	1.71	0.55
2:B:329:GLN:NE2	2:B:824:ASN:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:THR:C	2:B:607:LYS:H	2.13	0.55
2:B:317:THR:HG22	2:B:319:CYS:H	1.72	0.55
2:B:821:TYR:O	2:B:826:ALA:HB2	2.05	0.55
1:A:585:ARG:HA	1:A:590:LEU:HD12	1.87	0.55
2:B:386:CYS:O	2:B:390:ASN:N	2.39	0.55
2:B:606:ASP:HA	2:B:802:PRO:HG3	1.89	0.55
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.36	0.55
2:B:919:ILE:C	2:B:920:PHE:CD1	2.84	0.55
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.89	0.55
2:B:916:GLU:O	2:B:933:GLY:CA	2.52	0.55
2:B:389:CYS:O	2:B:390:ASN:HB2	2.07	0.54
1:A:310:ILE:HG21	1:A:354:GLN:HB2	1.89	0.54
2:B:889:GLN:HG2	2:B:891:LEU:CD2	2.36	0.54
2:B:522:LEU:HD21	2:B:525:GLY:HA3	1.90	0.54
1:A:113:GLN:HE21	1:A:114:PHE:HE2	1.51	0.54
1:A:258:LYS:HD3	1:A:305:GLU:HA	1.90	0.53
2:B:941:ILE:HG23	2:B:953:ILE:HD11	1.89	0.53
2:B:1025:HIS:HA	2:B:1028:ILE:HB	1.90	0.53
2:B:275:ASP:CB	2:B:295:LEU:HD12	2.37	0.53
2:B:403:LEU:HG	2:B:404:ASP:N	2.23	0.53
2:B:708:GLY:C	2:B:709:ILE:CG2	2.81	0.53
2:B:823:LYS:HE3	2:B:824:ASN:HD21	1.73	0.53
2:B:934:VAL:HG13	2:B:993:GLN:HB3	1.89	0.53
2:B:834:LEU:HD13	2:B:1021:LEU:HB3	1.90	0.53
2:B:891:LEU:N	2:B:891:LEU:CD2	2.73	0.52
2:B:945:PHE:HE2	2:B:990:ILE:HD13	1.74	0.52
2:B:396:PRO:HB2	2:B:398:PHE:CD1	2.45	0.52
2:B:409:ARG:O	2:B:412:HIS:HB2	2.09	0.52
2:B:288:THR:HB	2:B:291:GLN:HB2	1.89	0.52
2:B:462:ILE:O	2:B:466:LEU:HB2	2.10	0.52
2:B:641:GLN:HG2	2:B:642:TYR:H	1.75	0.52
1:A:686:GLN:NE2	1:A:690:ASP:OD1	2.33	0.52
2:B:388:PHE:HA	2:B:697:SER:HA	1.91	0.52
2:B:403:LEU:CG	2:B:404:ASP:N	2.73	0.51
2:B:726:LYS:HD2	2:B:876:THR:OG1	2.10	0.51
1:A:123:ARG:HG3	1:A:125:PRO:CD	2.40	0.51
2:B:384:TYR:CZ	2:B:393:ASN:HB2	2.45	0.51
2:B:396:PRO:CB	2:B:398:PHE:CE1	2.86	0.51
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.92	0.51
1:A:54:ILE:CG2	1:A:56:TYR:CZ	2.92	0.51
1:A:31:ALA:HA	1:A:34:MET:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:GLY:O	2:B:709:ILE:HG23	2.11	0.50
2:B:895:THR:HG23	2:B:896:LEU:N	2.25	0.50
2:B:380:GLY:HA2	2:B:403:LEU:HD22	1.93	0.50
2:B:492:ASN:C	2:B:494:VAL:H	2.19	0.50
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.94	0.50
2:B:706:PHE:CD1	2:B:706:PHE:N	2.72	0.50
2:B:823:LYS:HE3	2:B:824:ASN:ND2	2.27	0.50
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.93	0.49
1:A:642:ILE:HA	1:A:648:LEU:HD11	1.94	0.49
2:B:275:ASP:CB	2:B:295:LEU:CD1	2.89	0.49
1:A:35:VAL:HG21	1:A:552:ARG:CB	2.43	0.49
2:B:909:CYS:O	2:B:1007:GLU:HB2	2.12	0.49
2:B:823:LYS:HG3	2:B:824:ASN:HD22	1.78	0.49
1:A:118:GLU:HG3	1:A:495:ARG:CD	2.42	0.48
2:B:1032:LEU:O	2:B:1033:ASN:HB2	2.13	0.48
1:A:649:LEU:HD23	1:A:658:ILE:HG12	1.95	0.48
1:A:511:GLN:CD	1:A:511:GLN:H	2.21	0.48
2:B:268:PRO:HG2	2:B:887:TYR:CE1	2.48	0.48
2:B:705:PHE:O	2:B:706:PHE:CD1	2.66	0.48
2:B:874:VAL:CA	2:B:877:MET:HG3	2.38	0.48
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.95	0.48
2:B:601:LYS:H	2:B:859:ARG:HH12	1.61	0.48
1:A:35:VAL:HG21	1:A:552:ARG:HB3	1.95	0.48
2:B:386:CYS:O	2:B:390:ASN:CA	2.62	0.48
1:A:116:SER:HA	1:A:496:VAL:O	2.15	0.47
1:A:607:PHE:HD2	1:A:608:MET:HE2	1.79	0.47
2:B:518:VAL:HG21	2:B:560:PRO:HB3	1.97	0.47
1:A:560:TYR:HB3	1:A:568:PHE:HA	1.97	0.47
2:B:852:LYS:NZ	2:B:1006:VAL:O	2.34	0.47
1:A:114:PHE:HB3	1:A:117:ILE:CG2	2.44	0.47
2:B:461:LEU:HD11	2:B:675:LEU:HD11	1.96	0.47
1:A:231:GLN:HB2	1:A:236:ILE:HG13	1.96	0.47
2:B:583:SER:OG	2:B:584:SER:N	2.47	0.47
1:A:499:ILE:C	1:A:499:ILE:CD1	2.85	0.46
2:B:365:ASN:N	2:B:393:ASN:HD21	2.12	0.46
2:B:452:SER:O	2:B:456:ASN:ND2	2.49	0.46
1:A:49:PRO:CD	1:A:50:ASP:N	2.73	0.46
2:B:562:ILE:HB	2:B:622:LEU:HD21	1.98	0.46
2:B:446:MET:HE3	2:B:580:ILE:HG12	1.99	0.46
2:B:899:LYS:HD2	2:B:899:LYS:HA	1.67	0.45
2:B:996:GLN:C	2:B:998:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ASN:N	2:B:307:ASN:OD1	2.49	0.45
2:B:268:PRO:HG2	2:B:887:TYR:CZ	2.52	0.45
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.82	0.45
1:A:420:ILE:HD11	1:A:529:LEU:HD23	1.97	0.45
2:B:324:SER:N	2:B:734:HIS:HD2	2.14	0.45
1:A:116:SER:C	1:A:117:ILE:HG23	2.42	0.45
2:B:680:ASN:O	2:B:684:LYS:HG3	2.17	0.45
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.52	0.45
2:B:492:ASN:HA	2:B:556:THR:HG22	1.99	0.44
1:A:34:MET:HE3	1:A:34:MET:HB3	1.72	0.44
1:A:183:ILE:HG12	1:A:184:SER:N	2.31	0.44
1:A:744:THR:HG21	1:A:752:PHE:HD1	1.83	0.44
1:A:116:SER:HA	1:A:497:THR:HA	1.98	0.44
1:A:448:ILE:HD11	1:A:457:LEU:HD11	2.00	0.44
2:B:869:TYR:CZ	2:B:873:LEU:HD11	2.52	0.44
1:A:123:ARG:HG3	1:A:125:PRO:HD2	2.00	0.44
1:A:228:ARG:HA	1:A:231:GLN:HE21	1.83	0.44
2:B:467:LYS:HB3	2:B:538:HIS:CE1	2.53	0.44
2:B:543:GLN:HB3	2:B:547:MET:HE3	1.99	0.44
1:A:254:VAL:HG21	1:A:260:PRO:HG3	2.00	0.44
1:A:190:ARG:NH1	2:B:519:PHE:HB3	2.32	0.43
1:A:358:LEU:HD22	1:A:597:PRO:HB3	2.00	0.43
1:A:695:ILE:HD11	1:A:699:ARG:NH2	2.33	0.43
2:B:466:LEU:O	2:B:470:LEU:HG	2.17	0.43
2:B:692:MET:HB3	2:B:717:VAL:HB	1.99	0.43
1:A:266:VAL:HG22	1:A:298:PRO:HD2	2.00	0.43
1:A:546:LEU:HD21	1:A:584:LEU:HD23	1.99	0.43
2:B:404:ASP:CB	2:B:408:ARG:CB	2.96	0.43
1:A:55:GLN:HG2	1:A:120:VAL:HG21	2.01	0.43
1:A:123:ARG:HG3	1:A:125:PRO:HD3	2.00	0.43
2:B:823:LYS:CG	2:B:824:ASN:N	2.80	0.43
2:B:454:ILE:HD13	2:B:459:VAL:HG21	2.00	0.43
2:B:632:SER:HA	2:B:655:THR:OG1	2.19	0.43
2:B:711:MET:HE1	2:B:714:THR:O	2.18	0.43
1:A:22:ASN:HB2	1:A:516:SER:HB2	2.00	0.43
1:A:747:VAL:CG1	1:A:751:VAL:HB	2.48	0.43
2:B:948:PRO:HG2	2:B:952:HIS:ND1	2.34	0.43
1:A:35:VAL:HG22	1:A:549:GLN:NE2	2.33	0.43
1:A:189:PHE:HZ	1:A:204:LEU:HD21	1.84	0.43
1:A:19:PHE:CD2	1:A:40:ALA:HB2	2.54	0.43
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:GLN:HE22	2:B:986:MET:H	1.67	0.43
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.54	0.43
2:B:602:LEU:HD21	2:B:859:ARG:CB	2.48	0.42
1:A:360:MET:HE3	1:A:360:MET:HB2	1.92	0.42
1:A:570:PHE:CD1	1:A:575:SER:HB3	2.53	0.42
2:B:955:THR:O	2:B:958:THR:OG1	2.36	0.42
1:A:297:GLY:H	1:A:300:MET:HE2	1.85	0.42
2:B:305:GLN:O	2:B:306:GLY:C	2.60	0.42
2:B:892:PRO:HG2	2:B:895:THR:HG21	2.02	0.42
1:A:35:VAL:HG22	1:A:549:GLN:HE21	1.83	0.42
2:B:605:THR:C	2:B:607:LYS:N	2.78	0.42
2:B:822:ARG:CG	2:B:1028:ILE:HG23	2.47	0.42
1:A:668:ARG:HA	1:A:673:GLN:NE2	2.34	0.42
2:B:897:ASP:O	2:B:900:SER:CB	2.68	0.42
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.55	0.42
2:B:893:ILE:N	2:B:893:ILE:HD13	2.34	0.42
1:A:15:ASP:HB3	1:A:497:THR:CG2	2.50	0.42
2:B:633:VAL:HG13	2:B:652:PRO:HA	2.02	0.42
1:A:381:LEU:HA	1:A:702:MET:HE2	2.02	0.42
2:B:898:VAL:HG12	2:B:899:LYS:N	2.35	0.42
1:A:28:ARG:HD2	1:A:464:VAL:HA	2.02	0.41
2:B:495:LEU:HD21	2:B:561:VAL:HG22	2.02	0.41
1:A:172:MET:HE3	1:A:172:MET:HB2	1.94	0.41
1:A:18:ARG:NE	1:A:612:LEU:HD22	2.35	0.41
1:A:345:ILE:HG21	1:A:363:CYS:HB3	2.02	0.41
2:B:643:VAL:HG13	2:B:648:LEU:HD12	2.01	0.41
2:B:833:GLN:O	2:B:1025:HIS:NE2	2.53	0.41
1:A:627:SER:HB3	1:A:646:ARG:HG3	2.01	0.41
2:B:965:ASN:HB3	2:B:966:PRO:HD3	2.02	0.41
1:A:54:ILE:HG22	1:A:56:TYR:CD2	2.56	0.41
1:A:577:TYR:HB3	1:A:578:PRO:HD3	2.02	0.41
2:B:388:PHE:O	2:B:698:THR:N	2.50	0.41
2:B:794:ALA:O	2:B:798:VAL:HG23	2.21	0.41
2:B:904:PRO:O	2:B:904:PRO:CD	2.68	0.41
2:B:917:GLU:O	2:B:936:SER:HA	2.21	0.41
1:A:264:SER:HB2	1:A:294:ALA:HB2	2.02	0.41
2:B:321:PRO:HD3	2:B:777:LEU:HD21	2.02	0.41
2:B:601:LYS:HB3	2:B:605:THR:HG21	2.01	0.41
2:B:719:MET:SD	2:B:722:ILE:HD12	2.61	0.41
2:B:890:LEU:HD13	2:B:922:LEU:HD12	2.03	0.41
2:B:398:PHE:CD1	2:B:398:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:LEU:CD1	2:B:404:ASP:N	2.73	0.41
2:B:752:TYR:O	2:B:759:ARG:HD2	2.21	0.41
1:A:107:PRO:HB2	1:A:109:GLU:OE2	2.21	0.40
1:A:747:VAL:HG12	1:A:748:SER:O	2.21	0.40
2:B:368:LYS:HD3	2:B:368:LYS:HA	1.96	0.40
2:B:458:LEU:O	2:B:462:ILE:HG13	2.21	0.40
2:B:942:GLN:HG2	2:B:948:PRO:HA	2.03	0.40
1:A:244:LEU:HD23	1:A:247:LEU:HD12	2.04	0.40
2:B:405:HIS:C	2:B:406:ILE:HG13	2.46	0.40
2:B:822:ARG:HG2	2:B:1028:ILE:HG21	2.03	0.40
1:A:583:HIS:HA	1:A:586:ARG:HG2	2.04	0.40
2:B:409:ARG:O	2:B:412:HIS:CB	2.69	0.40
2:B:499:ASN:HA	2:B:525:GLY:O	2.21	0.40
2:B:703:THR:HG21	2:B:733:LYS:HB2	2.03	0.40
2:B:889:GLN:CG	2:B:891:LEU:HD21	2.48	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	708/765 (92%)	675 (95%)	30 (4%)	3 (0%)	30	62
2	B	760/767 (99%)	698 (92%)	59 (8%)	3 (0%)	30	62
3	C	1/8 (12%)	1 (100%)	0	0	100	100
All	All	1469/1540 (95%)	1374 (94%)	89 (6%)	6 (0%)	30	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	PRO

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Mol	Chain	Res	Type
2	B	966	PRO
1	A	125	PRO
2	B	965	ASN
2	B	904	PRO

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	624/666 (94%)	611 (98%)	13 (2%)	47	66
2	B	651/681 (96%)	626 (96%)	25 (4%)	29	56
3	C	3/7 (43%)	3 (100%)	0	100	100
All	All	1278/1354 (94%)	1240 (97%)	38 (3%)	36	60

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	54	ILE
1	A	118	GLU
1	A	201	GLN
1	A	455	THR
1	A	463	VAL
1	A	464	VAL
1	A	509	GLN
1	A	535	GLU
1	A	536	THR
1	A	722	VAL
1	A	742	ILE
1	A	745	ASP
2	B	279	ARG
2	B	307	ASN
2	B	313	ILE
2	B	323	THR
2	B	325	ASP

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Mol	Chain	Res	Type
2	B	398	PHE
2	B	406	ILE
2	B	492	ASN
2	B	526	PHE
2	B	528	VAL
2	B	536	VAL
2	B	567	GLU
2	B	602	LEU
2	B	633	VAL
2	B	643	VAL
2	B	661	LYS
2	B	680	ASN
2	B	691	ILE
2	B	714	THR
2	B	734	HIS
2	B	834	LEU
2	B	842	VAL
2	B	891	LEU
2	B	920	PHE
2	B	1028	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	A	387	GLN
1	A	549	GLN
1	A	583	HIS
1	A	610	GLN
1	A	673	GLN
2	B	329	GLN
2	B	365	ASN
2	B	385	GLN
2	B	390	ASN
2	B	393	ASN
2	B	543	GLN
2	B	613	GLN
2	B	672	GLN
2	B	734	HIS
2	B	800	HIS
2	B	824	ASN
2	B	979	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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	716/765 (93%)	-0.35	2 (0%) 90 75	60, 139, 207, 258	0
2	B	764/767 (99%)	-0.32	1 (0%) 92 85	86, 139, 234, 393	0
3	C	3/8 (37%)	0.46	0 100 100	291, 291, 302, 304	0
All	All	1483/1540 (96%)	-0.33	3 (0%) 91 81	60, 139, 217, 393	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	PHE	2.8
2	B	1023	CYS	2.3
1	A	362	CYS	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	ZN	B	1101	1/1	0.98	0.06	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	A	801	1/1	0.99	0.03	111,111,111,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.