



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 05:20 pm BST

PDB ID : 9FSK / pdb_00009fsk
Title : Crystal structure of the HECT domain of Smurf1
Authors : Ostermann, N.
Deposited on : 2024-06-21
Resolution : 2.75 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

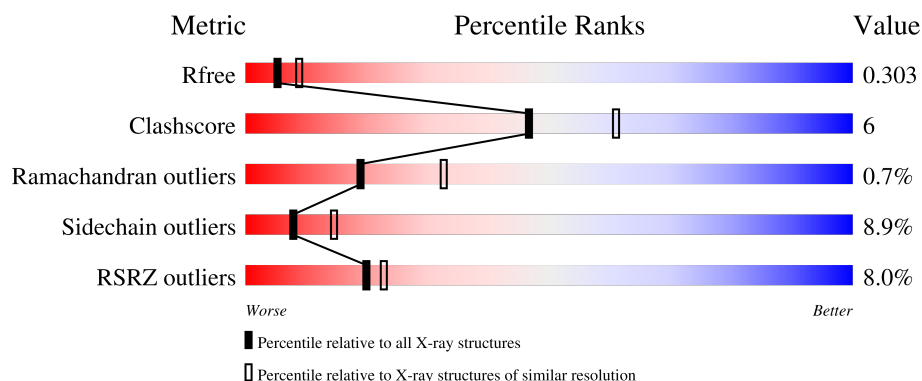
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	377	<div> <div>5%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	B	377	<div> <div>5%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	C	377	<div> <div>9%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>
1	D	377	<div> <div>13%</div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12302 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 E3 ubiquitin-protein ligase SMURF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			3060	1970	532	546	12			
1	B	371	Total	C	N	O	S	0	0	0
			3064	1973	532	547	12			
1	C	367	Total	C	N	O	S	0	0	0
			3019	1943	522	542	12			
1	D	358	Total	C	N	O	S	0	0	0
			2963	1910	513	528	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	GLY	-	expression tag	UNP Q9HCE7
A	376	PRO	-	expression tag	UNP Q9HCE7
B	375	GLY	-	expression tag	UNP Q9HCE7
B	376	PRO	-	expression tag	UNP Q9HCE7
C	375	GLY	-	expression tag	UNP Q9HCE7
C	376	PRO	-	expression tag	UNP Q9HCE7
D	375	GLY	-	expression tag	UNP Q9HCE7
D	376	PRO	-	expression tag	UNP Q9HCE7

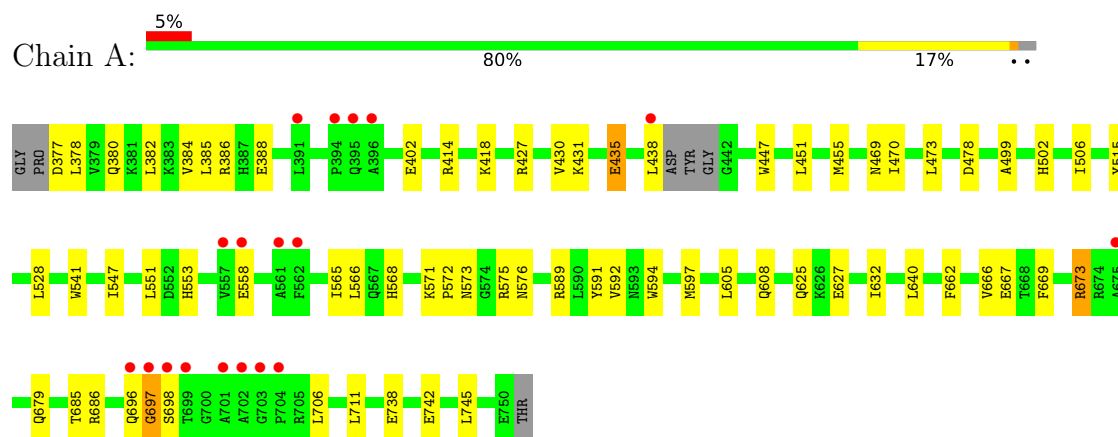
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	50	Total	O	0	0
			50	50		
2	C	40	Total	O	0	0
			40	40		
2	D	22	Total	O	0	0
			22	22		

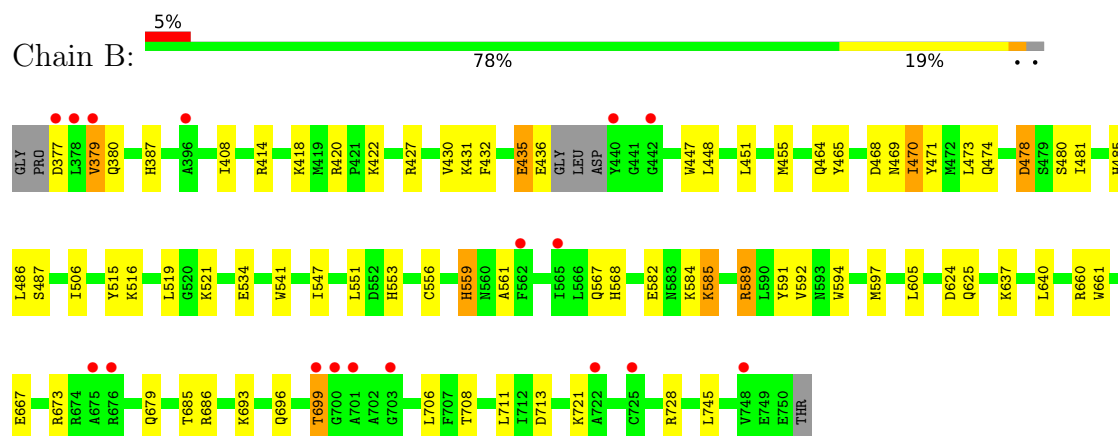
3 Residue-property plots [i](#)

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.

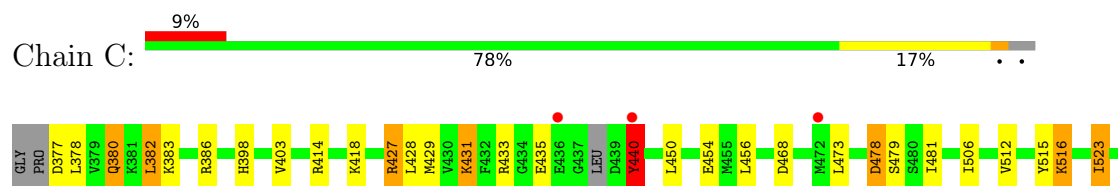
- Molecule 1: E3 ubiquitin-protein ligase SMURF1

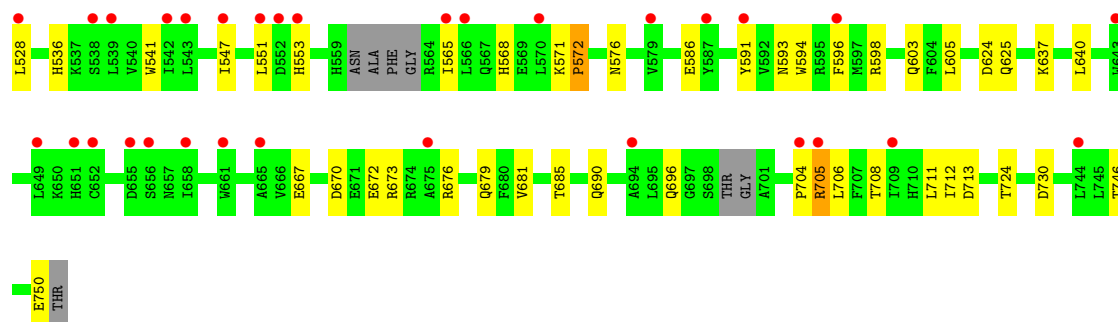


- Molecule 1: E3 ubiquitin-protein ligase SMURF1

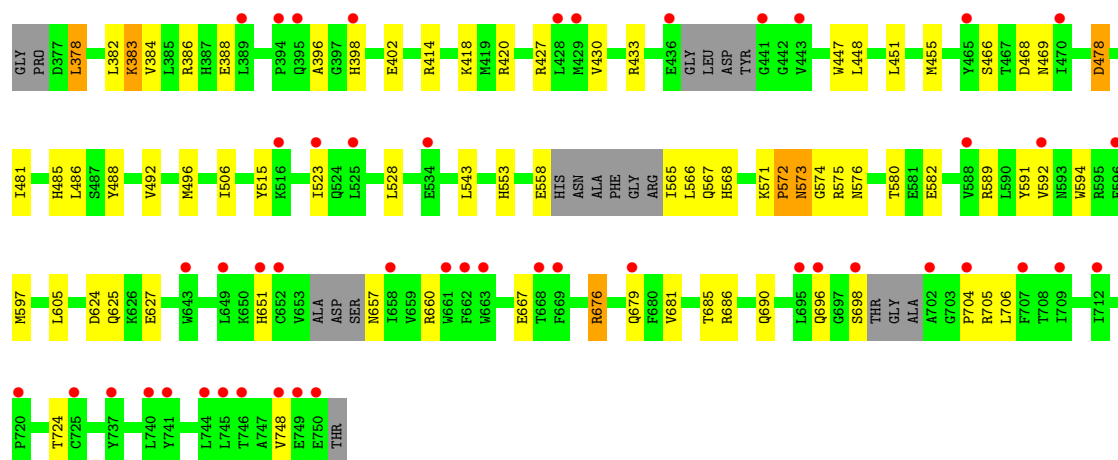
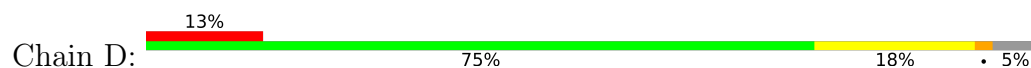


- Molecule 1: E3 ubiquitin-protein ligase SMURF1





● Molecule 1: E3 ubiquitin-protein ligase SMURF1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.16Å 74.32Å 161.06Å 90.00° 111.93° 90.00°	Depositor
Resolution (Å)	78.92 – 2.75 78.92 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (78.92-2.75) 98.9 (78.92-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.248 , 0.301 0.244 , 0.303	Depositor DCC
R_{free} test set	2419 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.83% 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](#)

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	0.48	0/3137	0.62	0/4242
1	B	0.44	0/3142	0.61	0/4249
1	C	0.39	0/3094	0.55	0/4183
1	D	0.39	0/3035	0.57	0/4099
All	All	0.43	0/12408	0.59	0/16773

There are no bond length outliers.

There are no bond angle outliers.

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	3060	0	3043	31	0
1	B	3064	0	3041	42	0
1	C	3019	0	2971	32	0
1	D	2963	0	2941	34	0
2	A	84	0	0	2	0
2	B	50	0	0	1	0
2	C	40	0	0	2	0
2	D	22	0	0	0	0
All	All	12302	0	11996	136	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 6.

All (136) 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:573:ASN:HD21	1:A:576:ASN:ND2	1.59	1.00
1:D:580:THR:HB	1:D:582:GLU:HG2	1.45	0.97
1:A:573:ASN:HD21	1:A:576:ASN:HD22	0.92	0.91
1:B:464:GLN:NE2	1:B:474:GLN:HE21	1.67	0.91
1:B:597:MET:HA	1:B:597:MET:HE2	1.61	0.82
1:D:398:HIS:NE2	1:D:427:ARG:NH1	2.29	0.80
1:A:573:ASN:ND2	1:A:576:ASN:HD22	1.77	0.80
1:D:657:ASN:HD21	1:D:660:ARG:HH21	1.27	0.78
1:B:464:GLN:NE2	1:B:474:GLN:NE2	2.34	0.75
1:C:431:LYS:HZ3	1:C:440:TYR:HD2	1.36	0.73
1:C:431:LYS:NZ	1:C:440:TYR:HD2	1.87	0.73
1:B:464:GLN:HE21	1:B:474:GLN:HE21	1.40	0.70
1:B:559:HIS:CE1	1:B:561:ALA:HB2	2.29	0.67
1:B:673:ARG:HE	1:B:745:LEU:HD11	1.60	0.66
1:A:673:ARG:HE	1:A:745:LEU:HD11	1.59	0.65
1:A:506:ILE:HD13	1:A:632:ILE:HG23	1.79	0.64
1:B:708:THR:HB	1:B:728:ARG:HG3	1.78	0.64
1:C:382:LEU:HB3	2:C:813:HOH:O	1.98	0.63
1:D:573:ASN:ND2	1:D:576:ASN:HD22	1.97	0.62
1:B:584:LYS:HE2	1:B:585:LYS:HZ1	1.63	0.62
1:B:464:GLN:HE21	1:B:474:GLN:NE2	1.96	0.62
1:B:516:LYS:NZ	1:B:625:GLN:HB2	2.16	0.61
1:B:515:TYR:HB2	1:B:625:GLN:HG2	1.82	0.61
1:B:465:TYR:CE2	1:D:420:ARG:NH1	2.69	0.60
1:C:512:VAL:HG12	1:C:516:LYS:HE2	1.85	0.59
1:A:418:LYS:NZ	2:A:803:HOH:O	2.35	0.58
1:A:669:PHE:HB3	1:A:673:ARG:HB3	1.84	0.58
1:B:551:LEU:HG	1:B:553:HIS:CD2	2.39	0.58
1:C:523:ILE:HD12	1:C:593:ASN:OD1	2.04	0.58
1:A:551:LEU:HG	1:A:553:HIS:CD2	2.39	0.57
1:D:696:GLN:HB2	1:D:704:PRO:HA	1.87	0.57
1:D:676:ARG:HB3	1:D:748:VAL:HG13	1.86	0.56
1:A:573:ASN:ND2	1:A:576:ASN:ND2	2.43	0.56
1:B:660:ARG:CZ	1:B:661:TRP:HE1	2.19	0.56
1:D:398:HIS:CE1	1:D:427:ARG:HH11	2.23	0.56
1:D:597:MET:HA	1:D:597:MET:HE2	1.87	0.56
1:A:738:GLU:O	1:A:742:GLU:HG2	2.07	0.55
1:C:398:HIS:CE1	1:C:427:ARG:HH11	2.25	0.55
1:A:528:LEU:HD22	1:A:592:VAL:HG22	1.89	0.54
1:B:584:LYS:HE3	1:B:585:LYS:HZ3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:HG	1:C:553:HIS:CD2	2.43	0.54
1:A:685:THR:HG23	1:A:686:ARG:HE	1.73	0.54
1:A:662:PHE:O	1:A:666:VAL:HG23	2.08	0.53
1:C:712:ILE:HD13	1:C:730:ASP:HB3	1.90	0.53
1:A:597:MET:HA	1:A:597:MET:HE2	1.90	0.53
1:B:673:ARG:NE	1:B:745:LEU:HD11	2.24	0.53
1:D:528:LEU:HD22	1:D:592:VAL:HG22	1.89	0.53
1:C:523:ILE:HG21	1:C:596:PHE:CE2	2.44	0.52
1:C:479:SER:OG	1:C:603:GLN:NE2	2.37	0.52
1:A:515:TYR:HB2	1:A:625:GLN:HG2	1.91	0.52
1:B:420:ARG:NE	1:B:422:LYS:HD2	2.24	0.52
1:C:705:ARG:HH11	1:C:705:ARG:HA	1.75	0.52
1:B:589:ARG:HA	1:B:592:VAL:HG12	1.92	0.51
1:B:485:HIS:CD2	1:B:486:LEU:HD22	2.45	0.51
1:B:568:HIS:CD2	1:B:594:TRP:NE1	2.79	0.51
1:D:515:TYR:HB2	1:D:625:GLN:HG2	1.91	0.51
1:B:414:ARG:O	1:B:418:LYS:HG3	2.11	0.51
1:B:660:ARG:NH1	1:B:661:TRP:CD1	2.79	0.50
1:D:398:HIS:HE2	1:D:427:ARG:NH1	2.09	0.50
1:B:660:ARG:CZ	1:B:661:TRP:NE1	2.75	0.50
1:C:672:GLU:HB3	1:C:676:ARG:HH21	1.76	0.50
1:B:465:TYR:HE2	1:D:420:ARG:NH1	2.09	0.50
1:B:568:HIS:CD2	1:B:594:TRP:CD1	3.00	0.50
1:C:515:TYR:HB2	1:C:625:GLN:HG2	1.93	0.50
1:B:430:VAL:HG11	1:B:447:TRP:CG	2.47	0.50
1:A:414:ARG:O	1:A:418:LYS:HG3	2.11	0.49
1:B:516:LYS:HZ1	1:B:625:GLN:HB2	1.77	0.49
1:B:673:ARG:HE	1:B:745:LEU:CD1	2.24	0.49
1:B:584:LYS:CE	1:B:585:LYS:NZ	2.74	0.49
1:A:499:ALA:HB3	1:A:506:ILE:HD11	1.93	0.49
1:B:451:LEU:O	1:B:455:MET:HG2	2.11	0.49
1:B:685:THR:HG23	1:B:686:ARG:HE	1.77	0.49
1:A:451:LEU:O	1:A:455:MET:HG2	2.13	0.49
1:A:430:VAL:HG11	1:A:447:TRP:CG	2.48	0.48
1:D:451:LEU:O	1:D:455:MET:HG2	2.13	0.48
1:A:568:HIS:CD2	1:A:594:TRP:NE1	2.82	0.48
1:B:556:CYS:SG	1:B:567:GLN:NE2	2.86	0.48
1:B:597:MET:HA	1:B:597:MET:CE	2.40	0.48
1:C:696:GLN:HB3	1:C:704:PRO:HA	1.95	0.48
1:D:685:THR:HG23	1:D:686:ARG:HE	1.79	0.48
1:A:568:HIS:CD2	1:A:594:TRP:CD1	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ARG:O	1:C:418:LYS:HG3	2.13	0.47
1:D:568:HIS:CD2	1:D:594:TRP:NE1	2.82	0.47
1:D:485:HIS:CD2	1:D:486:LEU:HD22	2.50	0.47
1:D:398:HIS:CD2	1:D:427:ARG:NH1	2.83	0.47
1:D:414:ARG:O	1:D:418:LYS:HG3	2.14	0.47
1:D:657:ASN:ND2	1:D:660:ARG:HH21	2.06	0.47
1:A:382:LEU:CD1	1:A:385:LEU:HD23	2.44	0.47
1:B:541:TRP:HZ3	1:B:547:ILE:HG22	1.79	0.46
1:C:450:LEU:O	1:C:454:GLU:HG2	2.15	0.46
1:A:378:LEU:HD13	1:A:627:GLU:HG2	1.97	0.46
1:C:673:ARG:HH21	1:C:676:ARG:HD3	1.80	0.46
1:D:568:HIS:CD2	1:D:594:TRP:CD1	3.04	0.46
1:C:398:HIS:CE1	1:C:427:ARG:NH1	2.83	0.46
1:B:584:LYS:HE3	1:B:585:LYS:NZ	2.30	0.46
1:C:568:HIS:CD2	1:C:594:TRP:NE1	2.84	0.46
1:A:696:GLN:O	1:A:697:GLY:O	2.33	0.46
1:B:673:ARG:HH22	1:D:396:ALA:HB1	1.82	0.45
1:D:478:ASP:O	1:D:481:ILE:HG12	2.17	0.45
1:A:384:VAL:O	1:A:388:GLU:HG2	2.16	0.45
1:A:541:TRP:HZ3	1:A:547:ILE:HG22	1.80	0.45
1:C:568:HIS:CD2	1:C:594:TRP:CD1	3.05	0.45
1:A:382:LEU:HD12	1:A:385:LEU:HD23	1.99	0.45
1:C:380:GLN:NE2	1:C:383:LYS:HD2	2.31	0.45
1:B:379:VAL:HG23	1:B:380:GLN:HE21	1.82	0.44
1:C:746:THR:O	1:C:750:GLU:HG2	2.18	0.44
1:D:430:VAL:HG11	1:D:447:TRP:CG	2.53	0.43
1:D:705:ARG:NE	1:D:705:ARG:HA	2.33	0.43
1:A:435:GLU:HB2	2:A:881:HOH:O	2.18	0.43
1:C:673:ARG:HA	1:C:676:ARG:HD2	2.01	0.43
1:C:681:VAL:O	1:C:724:THR:HA	2.19	0.43
1:D:571:LYS:HB2	1:D:572:PRO:HD2	2.01	0.43
1:C:478:ASP:O	1:C:481:ILE:HG12	2.18	0.43
1:D:402:GLU:HG2	1:D:433:ARG:HG2	2.01	0.43
1:C:456:LEU:HB3	1:C:473:LEU:HD11	2.01	0.43
1:A:571:LYS:HB2	1:A:572:PRO:HD2	2.01	0.43
1:B:480:SER:HB3	2:B:816:HOH:O	2.19	0.42
1:C:541:TRP:HZ3	1:C:547:ILE:HG22	1.84	0.42
1:C:679:GLN:HB2	1:C:685:THR:HG22	2.01	0.42
1:A:402:GLU:HA	1:A:431:LYS:O	2.20	0.42
1:A:502:HIS:O	1:A:698:SER:HB3	2.19	0.41
1:B:478:ASP:O	1:B:481:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:LEU:HD12	1:C:596:PHE:HE1	1.84	0.41
1:C:536:HIS:HD2	2:C:825:HOH:O	2.03	0.41
1:C:571:LYS:HB2	1:C:572:PRO:HD2	2.03	0.41
1:D:383:LYS:HA	1:D:383:LYS:HE2	2.03	0.41
1:D:492:VAL:O	1:D:496:MET:HG3	2.21	0.41
1:B:519:LEU:HG	1:B:521:LYS:HG3	2.03	0.41
1:D:378:LEU:HB3	1:D:627:GLU:OE2	2.21	0.41
1:C:403:VAL:C	1:C:433:ARG:HG3	2.42	0.41
1:B:408:ILE:HD12	1:B:432:PHE:HE1	1.86	0.41
1:D:488:TYR:O	1:D:492:VAL:HG23	2.22	0.40
1:D:681:VAL:O	1:D:724:THR:HA	2.21	0.40
1:D:384:VAL:O	1:D:388:GLU:HG2	2.22	0.40
1:B:516:LYS:HG2	1:B:625:GLN:HG3	2.04	0.40
1:D:466:SER:HB3	1:D:469:ASN:HB2	2.02	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	367/377 (97%)	345 (94%)	21 (6%)	1 (0%)	37	55
1	B	367/377 (97%)	339 (92%)	24 (6%)	4 (1%)	12	21
1	C	359/377 (95%)	340 (95%)	16 (4%)	3 (1%)	16	29
1	D	348/377 (92%)	324 (93%)	22 (6%)	2 (1%)	22	36
All	All	1441/1508 (96%)	1348 (94%)	83 (6%)	10 (1%)	19	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	697	GLY

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Mol	Chain	Res	Type
1	B	696	GLN
1	C	705	ARG
1	B	435	GLU
1	C	440	TYR
1	D	574	GLY
1	B	699	THR
1	D	572	PRO
1	B	470	ILE
1	C	572	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	334/338 (99%)	310 (93%)	24 (7%)	12	22
1	B	334/338 (99%)	300 (90%)	34 (10%)	6	10
1	C	327/338 (97%)	295 (90%)	32 (10%)	6	11
1	D	324/338 (96%)	296 (91%)	28 (9%)	8	15
All	All	1319/1352 (98%)	1201 (91%)	118 (9%)	8	14

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	ASP
1	A	380	GLN
1	A	386	ARG
1	A	427	ARG
1	A	435	GLU
1	A	438	LEU
1	A	469	ASN
1	A	470	ILE
1	A	473	LEU
1	A	478	ASP
1	A	558	GLU
1	A	565	ILE

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Mol	Chain	Res	Type
1	A	566	LEU
1	A	575	ARG
1	A	589	ARG
1	A	591	TYR
1	A	605	LEU
1	A	608	GLN
1	A	640	LEU
1	A	667	GLU
1	A	673	ARG
1	A	679	GLN
1	A	706	LEU
1	A	711	LEU
1	B	377	ASP
1	B	379	VAL
1	B	387	HIS
1	B	427	ARG
1	B	431	LYS
1	B	435	GLU
1	B	436	GLU
1	B	448	LEU
1	B	468	ASP
1	B	469	ASN
1	B	470	ILE
1	B	471	TYR
1	B	473	LEU
1	B	478	ASP
1	B	487	SER
1	B	506	ILE
1	B	534	GLU
1	B	559	HIS
1	B	582	GLU
1	B	585	LYS
1	B	589	ARG
1	B	591	TYR
1	B	605	LEU
1	B	624	ASP
1	B	637	LYS
1	B	640	LEU
1	B	667	GLU
1	B	679	GLN
1	B	693	LYS
1	B	699	THR

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Mol	Chain	Res	Type
1	B	706	LEU
1	B	711	LEU
1	B	713	ASP
1	B	721	LYS
1	C	377	ASP
1	C	378	LEU
1	C	380	GLN
1	C	382	LEU
1	C	386	ARG
1	C	427	ARG
1	C	428	LEU
1	C	429	MET
1	C	431	LYS
1	C	435	GLU
1	C	440	TYR
1	C	468	ASP
1	C	478	ASP
1	C	506	ILE
1	C	516	LYS
1	C	523	ILE
1	C	565	ILE
1	C	576	ASN
1	C	586	GLU
1	C	591	TYR
1	C	598	ARG
1	C	605	LEU
1	C	624	ASP
1	C	637	LYS
1	C	640	LEU
1	C	667	GLU
1	C	670	ASP
1	C	690	GLN
1	C	706	LEU
1	C	708	THR
1	C	711	LEU
1	C	713	ASP
1	D	378	LEU
1	D	382	LEU
1	D	383	LYS
1	D	386	ARG
1	D	448	LEU
1	D	468	ASP

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Mol	Chain	Res	Type
1	D	478	ASP
1	D	506	ILE
1	D	523	ILE
1	D	543	LEU
1	D	553	HIS
1	D	558	GLU
1	D	565	ILE
1	D	566	LEU
1	D	567	GLN
1	D	573	ASN
1	D	575	ARG
1	D	589	ARG
1	D	591	TYR
1	D	605	LEU
1	D	624	ASP
1	D	651	HIS
1	D	667	GLU
1	D	676	ARG
1	D	679	GLN
1	D	690	GLN
1	D	698	SER
1	D	706	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	GLN
1	A	395	GLN
1	A	464	GLN
1	A	568	HIS
1	A	576	ASN
1	A	608	GLN
1	B	380	GLN
1	B	392	GLN
1	B	393	GLN
1	B	464	GLN
1	B	469	ASN
1	B	567	GLN
1	B	568	HIS
1	B	679	GLN
1	B	696	GLN
1	C	380	GLN

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Mol	Chain	Res	Type
1	C	387	HIS
1	C	392	GLN
1	C	398	HIS
1	C	464	GLN
1	C	679	GLN
1	C	696	GLN
1	D	393	GLN
1	D	464	GLN
1	D	567	GLN
1	D	573	ASN
1	D	657	ASN
1	D	679	GLN
1	D	696	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](#)

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

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	371/377 (98%)	0.28	18 (4%) 36 38	26, 47, 81, 97	0
1	B	371/377 (98%)	0.56	17 (4%) 38 39	30, 61, 93, 108	0
1	C	367/377 (97%)	0.70	34 (9%) 16 18	27, 72, 128, 138	0
1	D	358/377 (94%)	0.97	48 (13%) 8 10	38, 83, 145, 163	0
All	All	1467/1508 (97%)	0.62	117 (7%) 20 23	26, 63, 126, 163	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	VAL	4.6
1	C	539	LEU	4.3
1	B	675	ALA	4.1
1	A	704	PRO	4.0
1	D	652	CYS	3.8
1	B	378	LEU	3.8
1	D	709	ILE	3.8
1	D	707	PHE	3.8
1	C	587	TYR	3.7
1	C	675	ALA	3.7
1	C	658	ILE	3.6
1	A	699	THR	3.5
1	D	750	GLU	3.5
1	D	525	LEU	3.5
1	C	538	SER	3.4
1	D	429	MET	3.4
1	D	749	GLU	3.4
1	D	695	LEU	3.2
1	D	741	TYR	3.2
1	A	698	SER	3.2
1	C	440	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	643	TRP	3.1
1	D	704	PRO	3.1
1	D	658	ILE	3.0
1	D	712	ILE	3.0
1	D	651	HIS	2.9
1	C	579	VAL	2.9
1	C	656	SER	2.9
1	D	592	VAL	2.9
1	D	702	ALA	2.9
1	C	744	LEU	2.9
1	B	700	GLY	2.8
1	C	651	HIS	2.8
1	D	696	GLN	2.8
1	A	696	GLN	2.8
1	D	679	GLN	2.7
1	C	643	TRP	2.7
1	D	596	PHE	2.7
1	A	703	GLY	2.7
1	D	470	ILE	2.7
1	A	557	VAL	2.7
1	B	565	ILE	2.7
1	C	543	LEU	2.6
1	C	551	LEU	2.6
1	D	516	LYS	2.6
1	C	596	PHE	2.6
1	D	441	GLY	2.6
1	D	698	SER	2.6
1	B	676	ARG	2.6
1	C	665	ALA	2.6
1	D	746	THR	2.6
1	C	542	ILE	2.6
1	D	428	LEU	2.5
1	B	379	VAL	2.5
1	D	748	VAL	2.5
1	D	661	TRP	2.5
1	C	570	LEU	2.5
1	D	740	LEU	2.5
1	D	720	PRO	2.5
1	D	465	TYR	2.5
1	C	704	PRO	2.4
1	D	398	HIS	2.4
1	D	725	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	377	ASP	2.4
1	A	396	ALA	2.4
1	B	722	ALA	2.4
1	B	725	CYS	2.4
1	C	552	ASP	2.4
1	D	389	LEU	2.4
1	B	440	TYR	2.4
1	B	703	GLY	2.4
1	C	528	LEU	2.4
1	D	534	GLU	2.3
1	D	745	LEU	2.3
1	B	562	PHE	2.3
1	A	675	ALA	2.3
1	A	701	ALA	2.3
1	B	442	GLY	2.3
1	C	472	MET	2.3
1	D	443	VAL	2.3
1	A	562	PHE	2.3
1	C	661	TRP	2.3
1	D	663	TRP	2.3
1	B	699	THR	2.2
1	D	588	VAL	2.2
1	D	523	ILE	2.2
1	A	702	ALA	2.2
1	C	694	ALA	2.2
1	C	649	LEU	2.2
1	C	709	ILE	2.2
1	A	438	LEU	2.2
1	C	566	LEU	2.2
1	C	436	GLU	2.2
1	D	668	THR	2.2
1	A	395	GLN	2.2
1	C	565	ILE	2.2
1	D	395	GLN	2.2
1	C	652	CYS	2.2
1	C	591	TYR	2.2
1	C	655	ASP	2.2
1	A	561	ALA	2.2
1	C	553	HIS	2.1
1	D	649	LEU	2.1
1	D	744	LEU	2.1
1	C	547	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	396	ALA	2.1
1	D	669	PHE	2.1
1	D	737	TYR	2.1
1	C	705	ARG	2.1
1	A	697	GLY	2.1
1	A	394	PRO	2.1
1	A	558	GLU	2.1
1	D	436	GLU	2.1
1	D	662	PHE	2.1
1	A	391	LEU	2.1
1	D	394	PRO	2.0
1	B	701	ALA	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 monosaccharides 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.