



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:10 AM UTC

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	:	4-5-2 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

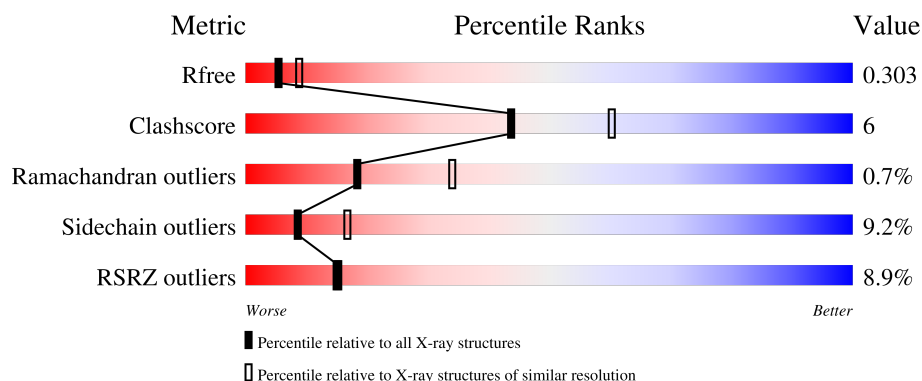
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	5% 78% 20% ..
1	B	377	5% 76% 20% ..
1	C	377	10% 76% 18% ...
1	D	377	15% 75% 18% • 5%

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

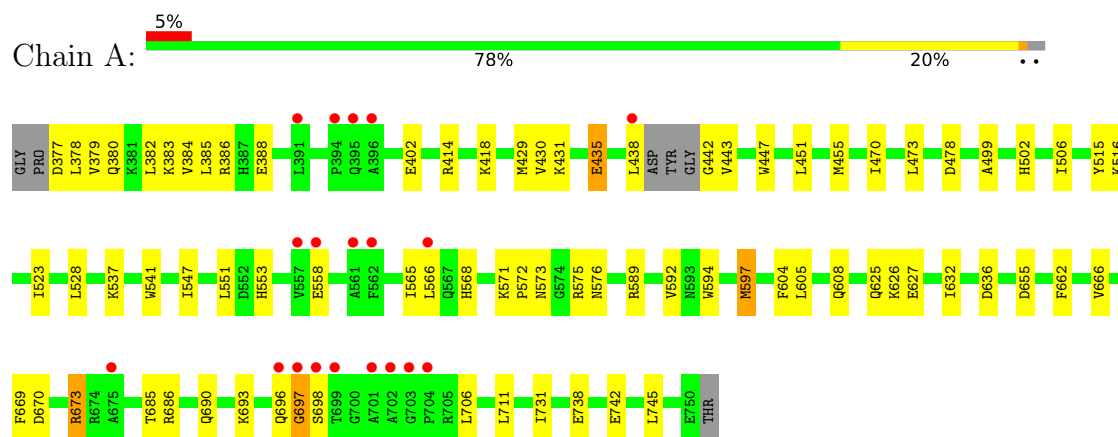
- Molecule 2 is water.

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		

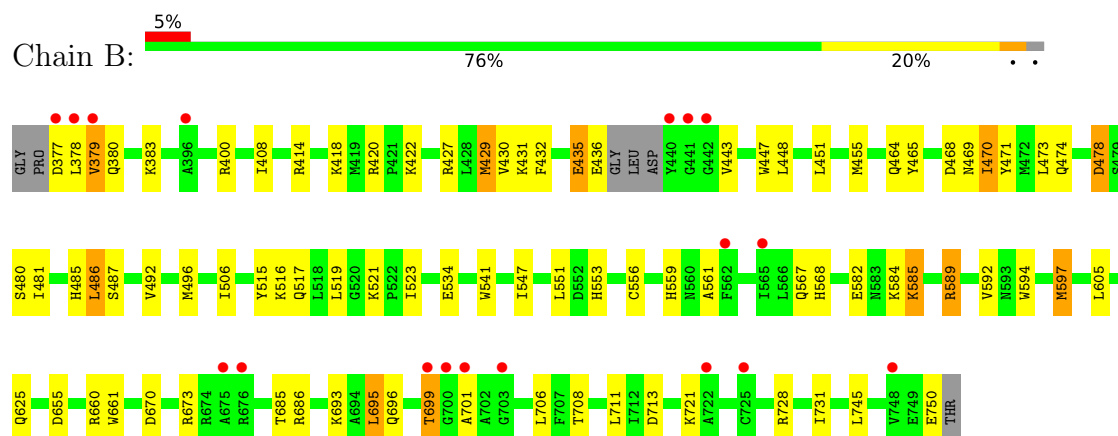
3 Residue-property plots [i](#)

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.

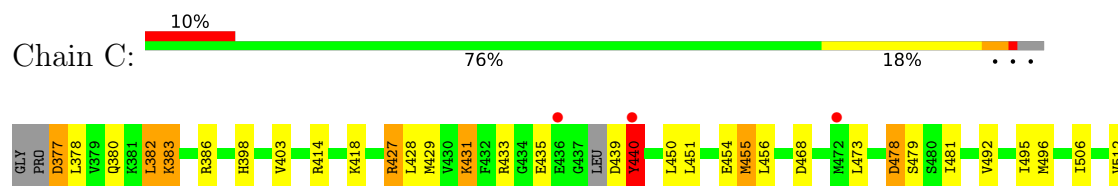
- Molecule 1: E3 ubiquitin-protein ligase SMURF1

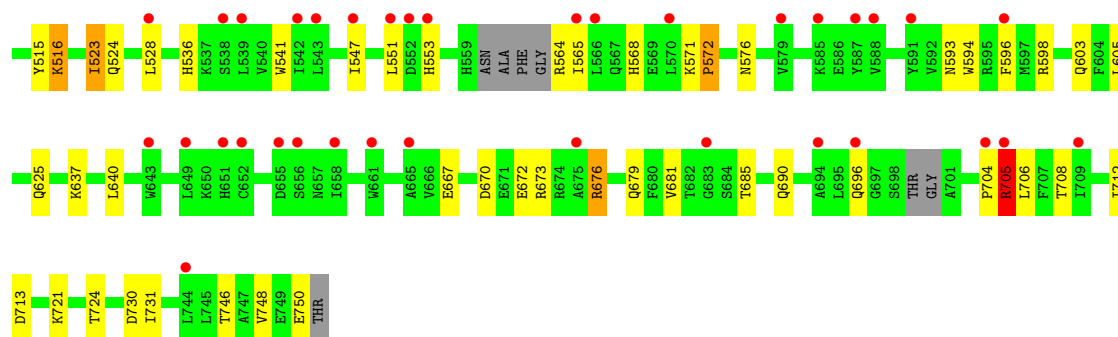


- Molecule 1: E3 ubiquitin-protein ligase SMURF1

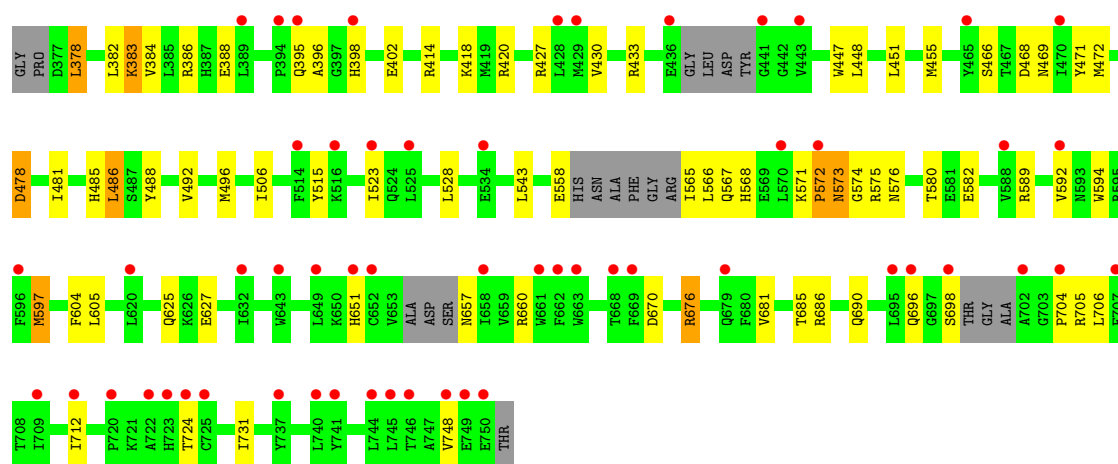
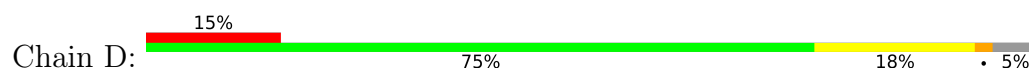


- Molecule 1: E3 ubiquitin-protein ligase SMURF1





● 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 , 67.6	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

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	0.82	0/3137	1.18	9/4242 (0.2%)
1	B	0.78	1/3142 (0.0%)	1.16	6/4249 (0.1%)
1	C	0.72	1/3094 (0.0%)	1.10	5/4183 (0.1%)
1	D	0.72	0/3035	1.10	2/4099 (0.0%)
All	All	0.76	2/12408 (0.0%)	1.13	22/16773 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	701	ALA	CA-C	7.28	1.62	1.52
1	C	455	MET	SD-CE	-5.98	1.64	1.79

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	ASP	CA-CB-CG	6.84	119.44	112.60
1	B	378	LEU	N-CA-C	6.81	118.36	111.07
1	A	670	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	443	VAL	N-CA-C	6.43	117.11	108.11
1	B	695	LEU	CA-C-N	6.08	133.16	121.54
1	B	695	LEU	C-N-CA	6.08	133.16	121.54
1	B	670	ASP	CA-CB-CG	6.07	118.67	112.60
1	D	731	ILE	N-CA-C	5.84	114.31	107.77
1	B	731	ILE	N-CA-C	5.80	114.26	107.77
1	D	670	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	439	ASP	CA-C-N	5.52	132.08	121.54
1	C	439	ASP	C-N-CA	5.52	132.08	121.54
1	C	731	ILE	N-CA-C	5.49	113.92	107.77
1	A	655	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	377	ASP	CA-C-N	5.37	128.87	120.82
1	C	377	ASP	C-N-CA	5.37	128.87	120.82
1	A	379	VAL	CA-C-N	5.35	127.71	120.65
1	A	379	VAL	C-N-CA	5.35	127.71	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	655	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	731	ILE	N-CA-C	5.31	113.72	107.77
1	A	442	GLY	CA-C-N	-5.02	116.56	123.14
1	A	442	GLY	C-N-CA	-5.02	116.56	123.14

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	3060	0	3043	33	0
1	B	3064	0	3041	45	0
1	C	3019	0	2971	35	0
1	D	2963	0	2941	37	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	147	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 (147) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:597:MET:HA	1:B:597:MET:HE2	1.76	0.67
1:B:559:HIS:CE1	1:B:561:ALA:HB2	2.29	0.67
1:C:431:LYS:HZ3	1:C:440:TYR:HD2	1.41	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:B:517:GLN:NE2	1:B:597:MET:HE3	2.11	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:C:451:LEU:HG	1:C:455:MET:HE3	1.85	0.57
1:A:551:LEU:HG	1:A:553:HIS:CD2	2.39	0.57
1:D:492:VAL:HG12	1:D:496:MET:HE3	1.86	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:A:597:MET:HE1	1:A:604:PHE:CB	2.36	0.55
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:597:MET:HA	1:B:597:MET:CE	2.40	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:516:LYS:HZ1	1:B:625:GLN:HB2	1.76	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:400:ARG:HH21	1:B:429:MET:HE2	1.77	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:673:ARG:HE	1:B:745:LEU:CD1	2.24	0.49
1:A:429:MET:HE2	1:A:431:LYS:HE2	1.94	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:492:VAL:HG12	1:B:496:MET:HE3	1.94	0.49
1:D:597:MET:HE1	1:D:604:PHE:CB	2.42	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:C:492:VAL:HG12	1:C:496:MET:HE3	1.94	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:403:VAL:C	1:C:433:ARG:HG3	2.42	0.45
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:D:471:TYR:HB2	1:D:472:MET:HE2	1.98	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:A:597:MET:HA	1:A:597:MET:HE2	1.98	0.44
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:455:MET:HE1	1:C:495:ILE:HG13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:469:ASN:C	1:D:471:TYR:H	2.29	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

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	367/377 (97%)	345 (94%)	21 (6%)	1 (0%)	36	56
1	B	367/377 (97%)	339 (92%)	24 (6%)	4 (1%)	11	22
1	C	359/377 (95%)	340 (95%)	16 (4%)	3 (1%)	16	30
1	D	348/377 (92%)	324 (93%)	22 (6%)	2 (1%)	21	38
All	All	1441/1508 (96%)	1348 (94%)	83 (6%)	10 (1%)	18	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	697	GLY
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%)	308 (92%)	26 (8%)	11	21
1	B	334/338 (99%)	300 (90%)	34 (10%)	7	14
1	C	327/338 (97%)	293 (90%)	34 (10%)	7	13
1	D	324/338 (96%)	297 (92%)	27 (8%)	10	19
All	All	1319/1352 (98%)	1198 (91%)	121 (9%)	8	17

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	ASP
1	A	380	GLN
1	A	383	LYS
1	A	386	ARG
1	A	435	GLU
1	A	438	LEU
1	A	470	ILE
1	A	473	LEU
1	A	478	ASP
1	A	516	LYS
1	A	523	ILE
1	A	537	LYS

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Mol	Chain	Res	Type
1	A	558	GLU
1	A	565	ILE
1	A	566	LEU
1	A	575	ARG
1	A	589	ARG
1	A	597	MET
1	A	605	LEU
1	A	608	GLN
1	A	626	LYS
1	A	673	ARG
1	A	690	GLN
1	A	693	LYS
1	A	706	LEU
1	A	711	LEU
1	B	377	ASP
1	B	379	VAL
1	B	383	LYS
1	B	427	ARG
1	B	429	MET
1	B	431	LYS
1	B	435	GLU
1	B	436	GLU
1	B	443	VAL
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	486	LEU
1	B	487	SER
1	B	506	ILE
1	B	523	ILE
1	B	534	GLU
1	B	582	GLU
1	B	585	LYS
1	B	589	ARG
1	B	597	MET
1	B	605	LEU
1	B	693	LYS
1	B	695	LEU

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Mol	Chain	Res	Type
1	B	699	THR
1	B	706	LEU
1	B	711	LEU
1	B	713	ASP
1	B	721	LYS
1	B	750	GLU
1	C	377	ASP
1	C	378	LEU
1	C	382	LEU
1	C	383	LYS
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	524	GLN
1	C	564	ARG
1	C	565	ILE
1	C	576	ASN
1	C	598	ARG
1	C	605	LEU
1	C	637	LYS
1	C	640	LEU
1	C	667	GLU
1	C	670	ASP
1	C	676	ARG
1	C	690	GLN
1	C	705	ARG
1	C	706	LEU
1	C	708	THR
1	C	713	ASP
1	C	721	LYS
1	C	748	VAL
1	D	378	LEU
1	D	382	LEU

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Mol	Chain	Res	Type
1	D	383	LYS
1	D	386	ARG
1	D	395	GLN
1	D	448	LEU
1	D	468	ASP
1	D	478	ASP
1	D	486	LEU
1	D	506	ILE
1	D	523	ILE
1	D	543	LEU
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	597	MET
1	D	605	LEU
1	D	651	HIS
1	D	676	ARG
1	D	690	GLN
1	D	698	SER
1	D	706	LEU
1	D	712	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	GLN
1	A	395	GLN
1	A	464	GLN
1	A	476	ASN
1	A	482	ASN
1	A	568	HIS
1	A	576	ASN
1	A	608	GLN
1	A	612	ASN
1	A	625	GLN
1	A	679	GLN
1	B	380	GLN
1	B	392	GLN

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Mol	Chain	Res	Type
1	B	393	GLN
1	B	464	GLN
1	B	469	ASN
1	B	482	ASN
1	B	567	GLN
1	B	568	HIS
1	B	612	ASN
1	B	679	GLN
1	B	696	GLN
1	C	380	GLN
1	C	387	HIS
1	C	392	GLN
1	C	398	HIS
1	C	464	GLN
1	C	476	ASN
1	C	482	ASN
1	C	504	HIS
1	C	568	HIS
1	C	612	ASN
1	C	625	GLN
1	C	646	ASN
1	C	679	GLN
1	C	696	GLN
1	D	392	GLN
1	D	393	GLN
1	D	482	ASN
1	D	553	HIS
1	D	567	GLN
1	D	568	HIS
1	D	573	ASN
1	D	576	ASN
1	D	612	ASN
1	D	625	GLN
1	D	657	ASN
1	D	679	GLN
1	D	696	GLN

5.3.3 RNA ⓘ

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%)	0.40	19 (5%) 33 33	26, 47, 81, 97	0
1	B	371/377 (98%)	0.68	18 (4%) 35 34	30, 61, 93, 108	0
1	C	367/377 (97%)	0.82	38 (10%) 11 11	27, 72, 128, 138	0
1	D	358/377 (94%)	1.09	56 (15%) 5 4	38, 83, 145, 163	0
All	All	1467/1508 (97%)	0.75	131 (8%) 15 15	26, 63, 126, 163	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	VAL	4.7
1	C	539	LEU	4.4
1	B	675	ALA	4.3
1	A	704	PRO	4.1
1	D	652	CYS	3.9
1	B	378	LEU	3.9
1	D	707	PHE	3.9
1	D	709	ILE	3.9
1	C	587	TYR	3.8
1	C	675	ALA	3.8
1	C	658	ILE	3.7
1	D	525	LEU	3.6
1	A	699	THR	3.6
1	D	750	GLU	3.6
1	D	429	MET	3.5
1	C	538	SER	3.5
1	D	749	GLU	3.4
1	D	741	TYR	3.3
1	D	695	LEU	3.3
1	C	440	TYR	3.3
1	D	643	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	698	SER	3.2
1	D	704	PRO	3.2
1	D	658	ILE	3.1
1	D	712	ILE	3.1
1	C	579	VAL	3.1
1	D	651	HIS	3.0
1	D	702	ALA	3.0
1	D	592	VAL	3.0
1	C	744	LEU	3.0
1	B	700	GLY	3.0
1	C	656	SER	2.9
1	C	651	HIS	2.9
1	D	696	GLN	2.9
1	D	596	PHE	2.9
1	A	696	GLN	2.8
1	C	643	TRP	2.8
1	A	703	GLY	2.8
1	D	679	GLN	2.8
1	D	470	ILE	2.8
1	A	557	VAL	2.8
1	B	565	ILE	2.8
1	C	543	LEU	2.8
1	C	551	LEU	2.8
1	C	596	PHE	2.7
1	D	441	GLY	2.7
1	C	665	ALA	2.7
1	D	516	LYS	2.7
1	C	542	ILE	2.7
1	D	698	SER	2.7
1	D	746	THR	2.7
1	D	428	LEU	2.6
1	B	379	VAL	2.6
1	B	676	ARG	2.6
1	D	748	VAL	2.6
1	D	661	TRP	2.6
1	C	570	LEU	2.6
1	D	465	TYR	2.6
1	D	740	LEU	2.6
1	D	720	PRO	2.6
1	D	725	CYS	2.6
1	C	704	PRO	2.6
1	D	398	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	396	ALA	2.5
1	B	722	ALA	2.5
1	B	725	CYS	2.5
1	B	377	ASP	2.5
1	D	389	LEU	2.5
1	B	440	TYR	2.5
1	B	703	GLY	2.5
1	C	528	LEU	2.5
1	C	552	ASP	2.5
1	B	562	PHE	2.5
1	D	745	LEU	2.5
1	B	442	GLY	2.5
1	A	562	PHE	2.5
1	A	675	ALA	2.5
1	A	701	ALA	2.5
1	C	661	TRP	2.4
1	D	663	TRP	2.4
1	C	472	MET	2.4
1	D	443	VAL	2.4
1	D	534	GLU	2.4
1	D	588	VAL	2.4
1	A	702	ALA	2.4
1	C	694	ALA	2.4
1	C	649	LEU	2.3
1	D	523	ILE	2.3
1	B	699	THR	2.3
1	A	438	LEU	2.3
1	C	566	LEU	2.3
1	C	709	ILE	2.3
1	C	652	CYS	2.3
1	C	565	ILE	2.3
1	C	591	TYR	2.3
1	D	668	THR	2.3
1	A	395	GLN	2.3
1	D	395	GLN	2.3
1	A	561	ALA	2.3
1	C	436	GLU	2.3
1	C	655	ASP	2.3
1	D	649	LEU	2.3
1	D	744	LEU	2.3
1	C	553	HIS	2.2
1	D	669	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	396	ALA	2.2
1	C	547	ILE	2.2
1	D	737	TYR	2.2
1	A	697	GLY	2.2
1	D	662	PHE	2.2
1	A	394	PRO	2.2
1	A	391	LEU	2.2
1	D	394	PRO	2.2
1	B	701	ALA	2.1
1	A	558	GLU	2.1
1	D	436	GLU	2.1
1	C	705	ARG	2.1
1	C	683	GLY	2.1
1	D	572	PRO	2.1
1	A	566	LEU	2.1
1	B	441	GLY	2.1
1	D	632	ILE	2.1
1	D	724	THR	2.1
1	C	696	GLN	2.1
1	D	620	LEU	2.1
1	D	723	HIS	2.1
1	C	588	VAL	2.1
1	D	514	PHE	2.1
1	D	570	LEU	2.0
1	C	585	LYS	2.0
1	D	722	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.