



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:30 PM UTC

PDB ID : 2IO1 / pdb_00002io1
Title : Crystal structure of human Senp2 in complex with preSUMO-3
Authors : Reverter, D.; Lima, C.D.
Deposited on : 2006-10-09
Resolution : 2.60 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

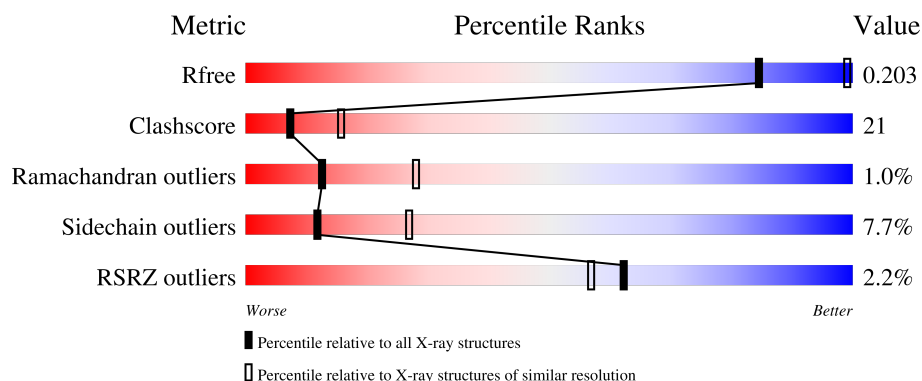
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	232	2% 57% 34% • •
1	C	232	58% 33% 6% •
1	E	232	4% 57% 34% 5% •
2	B	94	54% 28% • 14%
2	D	94	2% 53% 32% • 13%

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Mol	Chain	Length	Quality of chain
2	F	94	4% 49% 32% 5% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7816 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 Sentrin-specific protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			
1	C	224	Total	C	N	O	S	0	0	0
			1868	1201	326	331	10			
1	E	223	Total	C	N	O	S	0	0	0
			1860	1195	325	330	10			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	GLY	-	cloning artifact	UNP Q9HC62
A	359	SER	-	cloning artifact	UNP Q9HC62
A	360	HIS	-	cloning artifact	UNP Q9HC62
A	361	MET	-	cloning artifact	UNP Q9HC62
A	362	ALA	-	cloning artifact	UNP Q9HC62
A	363	SER	-	cloning artifact	UNP Q9HC62
A	548	SER	CYS	engineered mutation	UNP Q9HC62
C	358	GLY	-	cloning artifact	UNP Q9HC62
C	359	SER	-	cloning artifact	UNP Q9HC62
C	360	HIS	-	cloning artifact	UNP Q9HC62
C	361	MET	-	cloning artifact	UNP Q9HC62
C	362	ALA	-	cloning artifact	UNP Q9HC62
C	363	SER	-	cloning artifact	UNP Q9HC62
C	548	SER	CYS	engineered mutation	UNP Q9HC62
E	358	GLY	-	cloning artifact	UNP Q9HC62
E	359	SER	-	cloning artifact	UNP Q9HC62
E	360	HIS	-	cloning artifact	UNP Q9HC62
E	361	MET	-	cloning artifact	UNP Q9HC62
E	362	ALA	-	cloning artifact	UNP Q9HC62
E	363	SER	-	cloning artifact	UNP Q9HC62
E	548	SER	CYS	engineered mutation	UNP Q9HC62

- Molecule 2 is a protein called Small ubiquitin-related modifier 3 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total 648	C 401	N 116	O 127	S 4	0	0	0
2	D	82	Total 654	C 404	N 117	O 129	S 4	0	0	0
2	F	81	Total 648	C 401	N 116	O 127	S 4	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLY	-	cloning artifact	UNP P55854
B	11	SER	-	cloning artifact	UNP P55854
B	12	HIS	-	cloning artifact	UNP P55854
B	13	MET	-	cloning artifact	UNP P55854
D	10	GLY	-	cloning artifact	UNP P55854
D	11	SER	-	cloning artifact	UNP P55854
D	12	HIS	-	cloning artifact	UNP P55854
D	13	MET	-	cloning artifact	UNP P55854
F	10	GLY	-	cloning artifact	UNP P55854
F	11	SER	-	cloning artifact	UNP P55854
F	12	HIS	-	cloning artifact	UNP P55854
F	13	MET	-	cloning artifact	UNP P55854

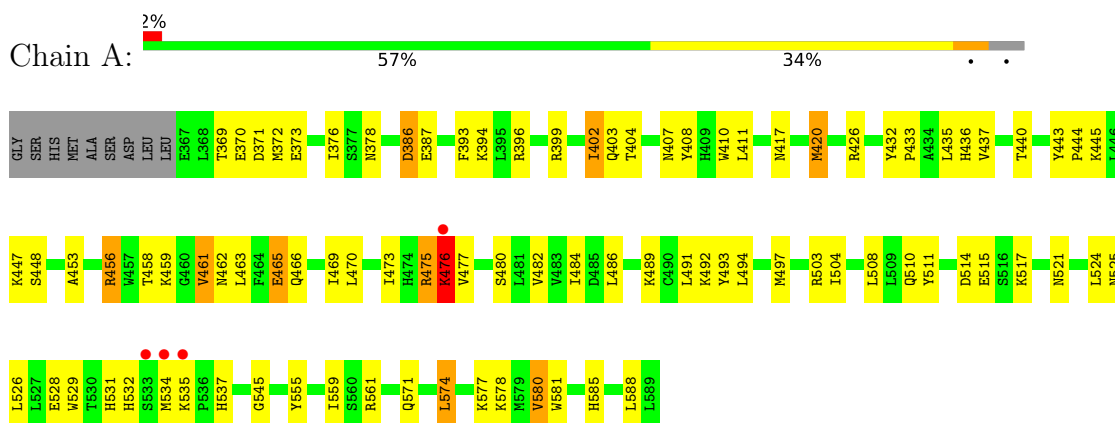
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total 74	O 74	0	0
3	B	27	Total 27	O 27	0	0
3	C	83	Total 83	O 83	0	0
3	D	31	Total 31	O 31	0	0
3	E	50	Total 50	O 50	0	0
3	F	13	Total 13	O 13	0	0

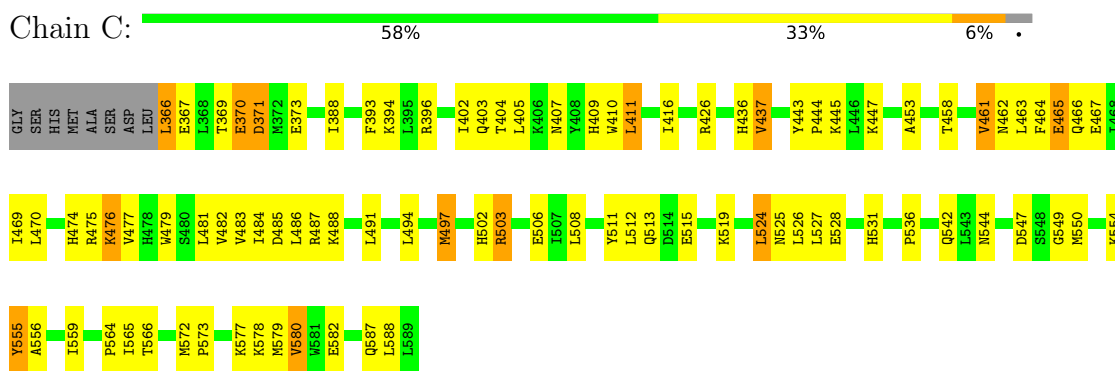
3 Residue-property plots

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.

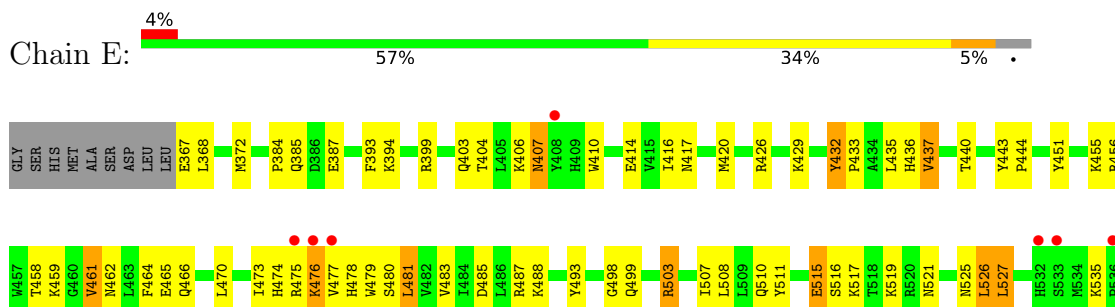
• Molecule 1: Sentrin-specific protease 2

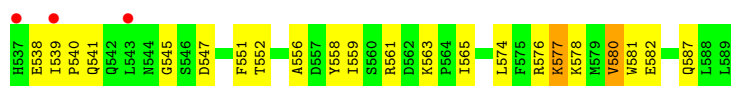


• Molecule 1: Sentrin-specific protease 2



• Molecule 1: Sentrin-specific protease 2





- Molecule 2: Small ubiquitin-related modifier 3 precursor

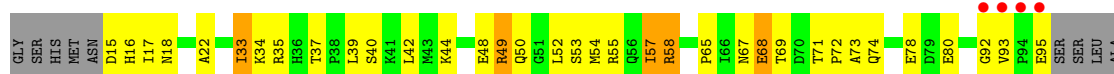


- Molecule 2: Small ubiquitin-related modifier 3 precursor



HIS
PHE

- Molecule 2: Small ubiquitin-related modifier 3 precursor



GLY
HIS
SER
PHE

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.98Å 143.36Å 134.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-2.60) 91.7 (20.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.230 0.205 , 0.203	Depositor DCC
R_{free} test set	2026 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7816	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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	0.60	0/1906	0.98	5/2567 (0.2%)
1	C	0.59	0/1914	1.00	6/2578 (0.2%)
1	E	0.56	0/1906	0.96	5/2567 (0.2%)
2	B	0.56	0/658	0.86	1/884 (0.1%)
2	D	0.57	0/664	0.91	2/892 (0.2%)
2	F	0.48	0/658	0.89	2/884 (0.2%)
All	All	0.57	0/7706	0.96	21/10372 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	ASP	N-CA-C	7.04	121.46	113.01
1	C	465	GLU	N-CA-C	-6.98	104.77	113.28
1	C	547	ASP	N-CA-C	6.90	121.41	112.92
1	A	555	TYR	N-CA-C	-6.67	103.63	111.03
1	A	404	THR	N-CA-C	-6.58	105.11	113.01
1	C	464	PHE	N-CA-C	6.52	120.95	113.19
1	C	481	LEU	N-CA-C	6.28	118.96	109.23
1	C	526	LEU	N-CA-C	6.25	119.75	111.75
1	E	475	ARG	N-CA-C	-6.19	100.76	110.36
1	C	555	TYR	N-CA-C	-5.67	105.02	111.14
2	F	22	ALA	N-CA-C	5.58	117.84	108.96
1	A	465	GLU	N-CA-C	-5.57	106.26	113.16
2	D	87	GLN	N-CA-C	-5.52	101.55	110.32
2	D	82	THR	N-CA-C	5.31	117.56	108.90
2	B	16	HIS	N-CA-C	5.29	117.52	108.90
1	E	481	LEU	N-CA-C	5.27	117.41	109.23
1	A	475	ARG	N-CA-C	-5.26	101.70	110.17
2	F	44	LYS	N-CA-C	-5.22	105.59	111.28
1	E	432	TYR	CA-C-N	5.19	125.19	119.90
1	E	432	TYR	C-N-CA	5.19	125.19	119.90
1	E	510	GLN	N-CA-C	-5.02	105.89	111.36

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	1860	0	1870	77	1
1	C	1868	0	1881	83	0
1	E	1860	0	1870	74	0
2	B	648	0	634	30	0
2	D	654	0	639	26	1
2	F	648	0	634	46	0
3	A	74	0	0	1	0
3	B	27	0	0	1	0
3	C	83	0	0	3	0
3	D	31	0	0	2	0
3	E	50	0	0	5	0
3	F	13	0	0	2	0
All	All	7816	0	7528	309	1

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 21.

All (309) 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:C:367:GLU:HB2	1:E:367:GLU:N	1.60	1.12
1:E:476:LYS:HD3	1:E:477:VAL:HG13	1.30	1.12
1:A:369:THR:HG22	1:A:371:ASP:H	1.23	1.04
2:F:71:THR:HG22	2:F:74:GLN:HG3	1.39	1.03
2:D:71:THR:HG22	2:D:74:GLN:H	1.28	0.98
1:E:462:ASN:ND2	1:E:465:GLU:HG3	1.78	0.97
1:E:462:ASN:HD22	1:E:465:GLU:HG3	1.26	0.97
2:B:71:THR:HG22	2:B:74:GLN:H	1.36	0.90
1:A:535:LYS:HB3	1:A:537:HIS:CE1	2.09	0.88
1:C:366:LEU:HD12	1:C:578:LYS:HD2	1.56	0.86
1:C:367:GLU:CB	1:E:367:GLU:N	2.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:SER:HB2	2:F:68:GLU:HB3	1.63	0.80
2:D:71:THR:HG21	3:D:131:HOH:O	1.83	0.79
1:E:403:GLN:HG2	1:E:406:LYS:HE3	1.66	0.77
1:C:447:LYS:HZ1	1:C:475:ARG:HH22	1.28	0.77
2:B:16:HIS:NE2	2:B:34:LYS:HE3	1.99	0.77
1:A:426:ARG:CZ	1:A:561:ARG:HD2	2.15	0.76
1:C:447:LYS:NZ	1:C:475:ARG:HH22	1.83	0.75
1:C:525:ASN:O	1:C:528:GLU:HG2	1.87	0.75
1:A:443:TYR:HB3	1:A:444:PRO:HD3	1.69	0.74
1:C:497:MET:HA	1:C:497:MET:HE2	1.68	0.74
2:B:71:THR:HG22	2:B:74:GLN:HG3	1.70	0.73
1:C:447:LYS:NZ	1:C:475:ARG:NH2	2.36	0.73
1:A:482:VAL:HG11	1:A:508:LEU:HD12	1.70	0.73
2:F:49:ARG:HG2	2:F:49:ARG:HH21	1.51	0.73
1:E:443:TYR:HB3	1:E:444:PRO:HD3	1.71	0.72
1:C:366:LEU:HD23	1:E:367:GLU:O	1.90	0.72
1:C:477:VAL:HA	2:D:91:GLY:HA2	1.71	0.71
1:A:437:VAL:HG22	1:A:470:LEU:HB2	1.73	0.71
2:D:71:THR:CG2	2:D:74:GLN:H	2.03	0.71
1:C:369:THR:HG22	1:C:371:ASP:H	1.56	0.70
1:A:456:ARG:HB3	1:A:456:ARG:HH11	1.57	0.69
1:A:497:MET:HE3	1:A:497:MET:HA	1.74	0.69
1:A:459:LYS:O	1:A:461:VAL:HG12	1.93	0.69
1:E:545:GLY:HA3	2:F:93:VAL:HG22	1.74	0.68
2:B:71:THR:HG23	2:B:73:ALA:H	1.59	0.67
2:D:15:ASP:CG	2:D:16:HIS:H	2.01	0.67
1:A:410:TRP:HE3	2:B:90:THR:HG22	1.60	0.67
2:F:16:HIS:NE2	2:F:34:LYS:HE3	2.11	0.66
2:D:40:SER:HA	2:D:43:MET:HE3	1.78	0.66
2:F:40:SER:CB	2:F:68:GLU:HB3	2.26	0.65
1:C:515:GLU:OE2	1:C:519:LYS:NZ	2.30	0.65
2:D:71:THR:HG22	2:D:74:GLN:N	2.08	0.65
1:A:426:ARG:C	1:A:426:ARG:HD2	2.21	0.65
1:C:497:MET:HE3	1:C:542:GLN:HG2	1.79	0.65
2:F:49:ARG:HG2	2:F:49:ARG:NH2	2.12	0.64
1:C:393:PHE:O	1:C:394:LYS:HB2	1.97	0.64
1:E:410:TRP:CD1	2:F:92:GLY:HA3	2.32	0.64
1:C:587:GLN:NE2	3:C:81:HOH:O	2.28	0.64
1:C:476:LYS:O	1:C:477:VAL:HG22	1.98	0.63
2:F:17:ILE:HD11	2:F:78:GLU:C	2.24	0.63
1:E:399:ARG:HG2	1:E:403:GLN:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:ARG:HD2	3:D:134:HOH:O	1.98	0.62
1:A:456:ARG:HB3	1:A:456:ARG:NH1	2.15	0.62
1:C:458:THR:O	1:C:461:VAL:HG13	1.99	0.62
1:E:436:HIS:HB2	1:E:466:GLN:HG3	1.80	0.62
1:C:467:GLU:OE1	1:C:487:ARG:HD3	2.00	0.62
1:A:535:LYS:HB3	1:A:537:HIS:NE2	2.14	0.61
2:B:19:LEU:HD12	2:B:33:ILE:HD11	1.83	0.61
1:E:519:LYS:HE2	3:E:214:HOH:O	2.00	0.61
1:A:386:ASP:OD2	2:B:55:ARG:NH1	2.34	0.61
2:F:40:SER:HB2	2:F:68:GLU:CB	2.30	0.61
1:C:550:MET:HE1	1:C:579:MET:HE3	1.83	0.61
2:B:15:ASP:O	2:B:34:LYS:HA	2.01	0.60
2:F:48:GLU:C	2:F:50:GLN:H	2.08	0.60
1:E:503:ARG:O	1:E:507:ILE:HG13	2.01	0.60
1:A:420:MET:CG	1:A:437:VAL:HG11	2.31	0.60
1:C:367:GLU:N	1:E:367:GLU:N	2.50	0.60
1:C:475:ARG:O	1:C:476:LYS:C	2.44	0.59
1:A:469:ILE:HB	1:A:484:ILE:HB	1.84	0.59
1:A:394:LYS:HB3	2:B:65:PRO:HG2	1.84	0.59
1:A:376:ILE:HG23	1:A:580:VAL:CG2	2.32	0.59
2:D:66:ILE:HG23	2:D:75:LEU:HD11	1.84	0.59
1:E:578:LYS:O	1:E:582:GLU:HG3	2.02	0.59
1:A:369:THR:HB	1:A:372:MET:HG3	1.83	0.59
1:A:492:LYS:HD3	1:A:534:MET:SD	2.43	0.59
2:F:71:THR:HG22	2:F:74:GLN:CG	2.24	0.58
1:A:491:LEU:HB2	1:A:531:HIS:HB3	1.86	0.58
1:C:491:LEU:O	1:C:531:HIS:HA	2.02	0.58
1:C:513:GLN:HA	1:C:524:LEU:HD22	1.86	0.58
1:C:497:MET:HE3	1:C:542:GLN:CG	2.33	0.57
1:E:414:GLU:OE2	1:E:414:GLU:HA	2.04	0.57
1:A:369:THR:HG22	1:A:371:ASP:N	2.07	0.57
1:E:385:GLN:NE2	2:F:55:ARG:NH1	2.51	0.57
1:A:545:GLY:O	2:B:93:VAL:HG22	2.03	0.57
2:B:71:THR:CG2	2:B:74:GLN:H	2.11	0.57
2:D:43:MET:HE1	2:D:68:GLU:HA	1.86	0.57
2:F:15:ASP:CG	2:F:16:HIS:H	2.11	0.57
1:A:503:ARG:HB3	3:A:99:HOH:O	2.04	0.57
2:B:71:THR:CG2	2:B:74:GLN:HG3	2.35	0.57
1:A:417:ASN:OD1	1:A:440:THR:HG23	2.04	0.57
1:A:482:VAL:HG11	1:A:508:LEU:CD1	2.34	0.57
2:B:42:LEU:C	2:B:42:LEU:HD23	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:TYR:HE1	1:E:515:GLU:HG2	1.69	0.56
2:F:71:THR:CG2	2:F:74:GLN:HG3	2.24	0.56
1:A:525:ASN:ND2	1:A:528:GLU:HG3	2.20	0.56
1:A:574:LEU:HD22	1:A:578:LYS:HG3	1.86	0.56
1:C:443:TYR:HB3	1:C:444:PRO:HD3	1.87	0.56
2:B:19:LEU:CD1	2:B:33:ILE:HD11	2.36	0.55
1:E:394:LYS:CB	2:F:65:PRO:HG2	2.36	0.55
1:E:481:LEU:HB2	1:E:552:THR:HG23	1.87	0.55
1:A:581:TRP:CE2	1:A:585:HIS:CD2	2.94	0.55
1:E:525:ASN:OD1	1:E:527:LEU:HB2	2.07	0.55
1:A:492:LYS:HD3	1:A:534:MET:HE2	1.88	0.55
2:B:17:ILE:HD11	2:B:78:GLU:O	2.07	0.55
1:A:475:ARG:O	1:A:476:LYS:C	2.49	0.55
1:C:436:HIS:HB2	1:C:466:GLN:HG3	1.89	0.55
1:E:540:PRO:HD2	1:E:565:ILE:HG21	1.89	0.55
2:F:39:LEU:HD21	2:F:72:PRO:HG3	1.89	0.55
1:A:387:GLU:OE2	1:A:399:ARG:NH1	2.40	0.55
2:D:18:ASN:OD1	2:D:32:LYS:HD2	2.07	0.55
1:C:388:ILE:N	1:C:388:ILE:HD12	2.23	0.54
1:C:483:VAL:HG21	1:C:559:ILE:HD13	1.89	0.54
2:D:44:LYS:O	2:D:48:GLU:HG2	2.06	0.54
1:C:474:HIS:HB2	1:C:479:TRP:CZ3	2.42	0.54
2:F:50:GLN:O	3:F:113:HOH:O	2.18	0.54
1:A:514:ASP:OD1	1:A:517:LYS:HE3	2.07	0.54
1:C:369:THR:HG22	1:C:371:ASP:N	2.22	0.54
1:C:447:LYS:HZ2	1:C:475:ARG:NH2	2.06	0.54
1:C:564:PRO:O	1:C:566:THR:HG23	2.08	0.53
1:E:540:PRO:HA	3:E:262:HOH:O	2.08	0.53
1:E:577:LYS:O	1:E:580:VAL:HG13	2.09	0.53
2:B:78:GLU:OE2	2:B:78:GLU:HA	2.09	0.53
2:B:40:SER:HB2	2:B:68:GLU:HB3	1.91	0.53
1:E:462:ASN:HD22	1:E:465:GLU:CG	2.12	0.53
1:E:473:ILE:HB	1:E:480:SER:HB3	1.91	0.53
1:A:508:LEU:O	1:A:511:TYR:HB3	2.09	0.53
1:E:508:LEU:O	1:E:511:TYR:HB3	2.09	0.52
1:E:547:ASP:O	1:E:551:PHE:HD1	1.92	0.52
1:E:420:MET:HG3	1:E:437:VAL:CG2	2.40	0.52
1:E:476:LYS:HD3	1:E:477:VAL:CG1	2.21	0.52
2:F:48:GLU:O	2:F:50:GLN:N	2.43	0.52
1:A:473:ILE:HD13	1:A:504:ILE:HG21	1.90	0.52
1:E:384:PRO:HB2	1:E:387:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ASN:ND2	2:B:32:LYS:HG2	2.25	0.52
1:C:410:TRP:HB2	2:D:90:THR:CG2	2.40	0.52
1:C:497:MET:HA	1:C:497:MET:CE	2.40	0.52
2:F:54:MET:HA	2:F:57:ILE:CD1	2.40	0.52
1:E:480:SER:HG	1:E:493:TYR:HH	1.58	0.51
2:B:17:ILE:HG22	2:B:33:ILE:O	2.10	0.51
1:C:477:VAL:HG23	1:C:477:VAL:O	2.10	0.51
1:C:577:LYS:HB2	1:C:577:LYS:NZ	2.25	0.51
1:E:517:LYS:O	1:E:521:ASN:HA	2.11	0.51
1:A:459:LYS:HE3	2:B:62:ASP:OD2	2.11	0.51
1:E:399:ARG:CG	1:E:403:GLN:NE2	2.74	0.51
1:E:565:ILE:H	1:E:565:ILE:HD12	1.76	0.51
1:A:426:ARG:NH2	1:A:561:ARG:HD2	2.26	0.50
2:F:71:THR:HG23	2:F:73:ALA:H	1.76	0.50
1:E:393:PHE:O	1:E:394:LYS:HB2	2.11	0.50
1:E:474:HIS:HB2	1:E:479:TRP:CZ3	2.47	0.50
1:E:535:LYS:H	1:E:538:GLU:CD	2.19	0.50
1:E:394:LYS:HB2	2:F:65:PRO:HG2	1.93	0.50
2:B:90:THR:HG21	3:B:112:HOH:O	2.10	0.50
2:F:71:THR:CG2	2:F:74:GLN:H	2.25	0.50
1:A:492:LYS:HG2	1:A:494:LEU:CD1	2.42	0.49
1:E:435:LEU:HD11	1:E:470:LEU:HG	1.94	0.49
2:D:15:ASP:CG	2:D:16:HIS:N	2.69	0.49
1:E:515:GLU:OE2	1:E:519:LYS:NZ	2.38	0.49
2:F:42:LEU:HD23	2:F:42:LEU:C	2.38	0.49
1:A:378:ASN:O	1:A:399:ARG:NH2	2.46	0.49
1:C:469:ILE:HD11	1:C:486:LEU:HD11	1.94	0.49
2:F:49:ARG:HG2	2:F:49:ARG:O	2.12	0.49
2:F:53:SER:O	2:F:57:ILE:HD12	2.11	0.49
2:F:52:LEU:HD13	2:F:57:ILE:HG21	1.94	0.48
2:B:57:ILE:C	2:B:58:ARG:HG2	2.38	0.48
1:A:376:ILE:HG23	1:A:580:VAL:HG21	1.93	0.48
1:C:550:MET:O	1:C:554:LYS:HG2	2.14	0.48
1:C:485:ASP:OD2	1:C:488:LYS:HE3	2.13	0.48
2:D:60:ARG:HD2	2:D:65:PRO:HA	1.94	0.48
2:F:34:LYS:HB2	2:F:37:THR:OG1	2.12	0.48
1:A:426:ARG:NH1	1:A:561:ARG:HD2	2.28	0.48
2:B:17:ILE:HG12	2:B:18:ASN:N	2.29	0.48
2:B:39:LEU:CD2	2:B:42:LEU:HD13	2.42	0.48
2:D:15:ASP:O	2:D:34:LYS:HA	2.13	0.48
1:C:503:ARG:HH11	1:C:503:ARG:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:GLN:HG2	2:D:88:GLN:OE1	2.13	0.48
1:A:493:TYR:C	1:A:494:LEU:HD12	2.39	0.47
1:A:489:LYS:O	1:A:529:TRP:HA	2.14	0.47
1:E:511:TYR:CZ	1:E:515:GLU:HG3	2.50	0.47
1:C:369:THR:HG21	3:E:184:HOH:O	2.14	0.47
1:C:404:THR:HB	1:C:410:TRP:O	2.14	0.47
1:A:394:LYS:CB	2:B:65:PRO:HG2	2.44	0.47
1:C:555:TYR:O	1:C:559:ILE:HG13	2.15	0.47
1:E:367:GLU:O	1:E:368:LEU:HD23	2.15	0.47
1:E:432:TYR:HB3	1:E:433:PRO:HD2	1.97	0.47
1:C:407:ASN:O	1:C:409:HIS:HD2	1.97	0.47
1:C:484:ILE:HG21	1:C:512:LEU:HD11	1.97	0.47
1:A:466:GLN:O	1:A:486:LEU:HD12	2.15	0.47
1:C:394:LYS:HB3	2:D:65:PRO:HG2	1.96	0.47
1:E:480:SER:OG	1:E:493:TYR:CZ	2.65	0.47
2:F:54:MET:HA	2:F:57:ILE:HD11	1.97	0.47
2:F:67:ASN:HB3	3:F:108:HOH:O	2.14	0.47
1:A:447:LYS:O	1:A:447:LYS:HG2	2.15	0.47
1:A:393:PHE:O	1:A:394:LYS:HB2	2.14	0.46
1:E:483:VAL:HG11	1:E:559:ILE:HG21	1.96	0.46
1:C:572:MET:N	1:C:573:PRO:CD	2.78	0.46
1:E:459:LYS:O	1:E:459:LYS:HG2	2.14	0.46
1:E:432:TYR:HB3	1:E:433:PRO:CD	2.45	0.46
2:B:59:PHE:O	2:B:60:ARG:HD2	2.15	0.46
1:A:525:ASN:HD22	1:A:528:GLU:HG3	1.80	0.46
1:C:437:VAL:HG22	1:C:470:LEU:HB2	1.97	0.46
2:F:17:ILE:HG12	2:F:18:ASN:N	2.30	0.46
1:A:436:HIS:HB2	1:A:466:GLN:HG3	1.98	0.46
1:E:385:GLN:HE22	2:F:55:ARG:NH1	2.14	0.46
1:A:426:ARG:HG3	1:A:588:LEU:HD12	1.98	0.46
2:B:71:THR:HG23	2:B:73:ALA:N	2.28	0.46
1:E:394:LYS:HB3	2:F:65:PRO:HG2	1.97	0.46
2:D:44:LYS:HE3	2:D:68:GLU:OE2	2.15	0.46
1:A:475:ARG:O	1:A:477:VAL:N	2.49	0.46
1:E:426:ARG:HD2	1:E:426:ARG:C	2.40	0.46
1:A:435:LEU:HD11	1:A:470:LEU:HG	1.97	0.46
1:C:426:ARG:HG3	1:C:426:ARG:HH11	1.81	0.46
1:A:376:ILE:HG23	1:A:580:VAL:HG22	1.98	0.45
1:C:536:PRO:HD2	3:C:75:HOH:O	2.14	0.45
1:E:527:LEU:HD12	1:E:527:LEU:HA	1.83	0.45
1:C:572:MET:HB3	3:C:135:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:LYS:HD2	2:F:34:LYS:N	2.31	0.45
2:F:48:GLU:C	2:F:50:GLN:N	2.74	0.45
1:E:420:MET:HG3	1:E:437:VAL:HG21	1.96	0.45
1:A:492:LYS:HD3	1:A:534:MET:CE	2.46	0.45
1:C:470:LEU:HD13	1:C:556:ALA:HB1	1.97	0.45
1:C:403:GLN:C	1:C:405:LEU:H	2.24	0.45
1:C:469:ILE:HB	1:C:484:ILE:HB	1.99	0.45
1:C:476:LYS:O	1:C:477:VAL:CG2	2.65	0.45
1:C:582:GLU:HB3	1:C:588:LEU:HD23	1.98	0.45
2:D:17:ILE:HG12	2:D:79:ASP:HA	1.99	0.45
1:C:394:LYS:CB	2:D:65:PRO:HG2	2.47	0.45
1:C:410:TRP:HE3	2:D:90:THR:CG2	2.29	0.45
1:C:483:VAL:HG11	1:C:559:ILE:HG21	1.99	0.45
1:E:385:GLN:HE22	2:F:55:ARG:HH11	1.63	0.45
1:A:396:ARG:NH1	1:A:396:ARG:HG2	2.32	0.45
1:C:463:LEU:HD23	1:C:463:LEU:HA	1.74	0.44
1:E:410:TRP:CG	2:F:92:GLY:HA3	2.52	0.44
1:A:473:ILE:CD1	1:A:504:ILE:HG21	2.46	0.44
1:A:432:TYR:HB3	1:A:433:PRO:CD	2.48	0.44
1:A:445:LYS:HE3	1:A:453:ALA:HB1	2.00	0.44
1:A:396:ARG:HG2	1:A:396:ARG:HH11	1.82	0.44
1:A:420:MET:HG3	1:A:437:VAL:HG21	1.99	0.44
1:C:369:THR:CG2	3:E:184:HOH:O	2.66	0.44
1:C:426:ARG:C	1:C:426:ARG:HD2	2.42	0.44
2:F:71:THR:HG23	2:F:73:ALA:N	2.33	0.44
1:C:369:THR:CG2	1:C:370:GLU:N	2.80	0.44
1:E:470:LEU:HD13	1:E:556:ALA:HB1	2.00	0.44
1:C:482:VAL:HG11	1:C:508:LEU:HD13	1.99	0.44
1:C:544:ASN:OD1	1:C:544:ASN:C	2.61	0.44
1:A:420:MET:HG2	1:A:437:VAL:HG11	1.99	0.44
2:B:60:ARG:HD2	2:B:65:PRO:HA	2.00	0.44
1:C:411:LEU:HG	1:C:549:GLY:HA3	1.99	0.43
2:F:33:ILE:HD13	2:F:33:ILE:H	1.83	0.43
2:F:33:ILE:CG2	2:F:42:LEU:HD12	2.48	0.43
1:C:416:ILE:HD12	1:C:479:TRP:CE2	2.53	0.43
1:C:485:ASP:OD2	1:C:488:LYS:CE	2.66	0.43
1:C:511:TYR:CZ	1:C:515:GLU:HG3	2.54	0.43
1:C:577:LYS:O	1:C:580:VAL:HG13	2.19	0.43
1:E:558:TYR:HB3	1:E:563:LYS:O	2.18	0.43
2:F:15:ASP:HB3	2:F:35:ARG:HD3	2.01	0.43
1:C:369:THR:O	1:C:373:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ASN:OD1	1:E:440:THR:HG23	2.18	0.43
2:F:68:GLU:H	2:F:68:GLU:HG2	1.40	0.43
1:C:411:LEU:N	1:C:411:LEU:HD23	2.33	0.43
1:E:485:ASP:OD2	1:E:488:LYS:HE2	2.18	0.43
1:A:402:ILE:HA	1:A:402:ILE:HD13	1.68	0.43
1:A:432:TYR:HB3	1:A:433:PRO:HD2	2.00	0.43
1:A:407:ASN:O	1:A:408:TYR:HB2	2.19	0.43
1:A:426:ARG:HG3	1:A:426:ARG:HH11	1.83	0.43
1:E:404:THR:HB	1:E:410:TRP:O	2.18	0.42
1:E:577:LYS:HB2	1:E:577:LYS:NZ	2.34	0.42
1:A:410:TRP:HB3	2:B:90:THR:HG23	1.99	0.42
2:B:71:THR:HG22	2:B:74:GLN:CG	2.47	0.42
1:E:456:ARG:NH2	3:E:88:HOH:O	2.51	0.42
2:F:15:ASP:CG	2:F:16:HIS:N	2.77	0.42
1:C:416:ILE:HD12	1:C:479:TRP:CZ2	2.55	0.42
1:E:539:ILE:HG13	1:E:541:GLN:NE2	2.35	0.42
1:E:565:ILE:HD12	1:E:565:ILE:N	2.33	0.42
1:C:445:LYS:HE3	1:C:453:ALA:HB1	2.00	0.42
1:A:535:LYS:H	1:A:535:LYS:HG3	1.68	0.42
1:C:403:GLN:C	1:C:405:LEU:N	2.78	0.42
1:E:426:ARG:CZ	1:E:561:ARG:HD2	2.50	0.42
1:A:399:ARG:O	1:A:403:GLN:HG3	2.20	0.42
1:A:510:GLN:NE2	1:A:510:GLN:HA	2.35	0.42
1:A:372:MET:O	1:A:376:ILE:HG13	2.19	0.42
1:C:565:ILE:N	1:C:565:ILE:HD13	2.34	0.42
2:F:71:THR:HG22	2:F:74:GLN:H	1.83	0.42
1:C:525:ASN:HB3	1:C:528:GLU:CD	2.44	0.42
1:A:475:ARG:NH1	1:A:493:TYR:OH	2.53	0.41
1:E:464:PHE:CZ	1:E:516:SER:HB2	2.55	0.41
2:D:61:PHE:O	2:D:62:ASP:HB2	2.20	0.41
1:A:369:THR:CG2	1:A:370:GLU:N	2.82	0.41
1:A:387:GLU:HG3	1:E:429:LYS:HB2	2.02	0.41
1:E:372:MET:HE3	1:E:581:TRP:CE2	2.56	0.41
2:F:15:ASP:O	2:F:34:LYS:HG3	2.20	0.41
1:A:492:LYS:HG2	1:A:494:LEU:HD11	2.01	0.41
1:E:526:LEU:HD23	1:E:526:LEU:HA	1.79	0.41
1:C:477:VAL:HA	2:D:90:THR:O	2.20	0.41
2:D:42:LEU:HD23	2:D:42:LEU:C	2.46	0.41
2:F:57:ILE:C	2:F:58:ARG:HG2	2.45	0.41
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.93	0.41
1:C:388:ILE:HD12	1:C:388:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:TYR:OH	1:C:515:GLU:HG3	2.20	0.41
1:E:458:THR:O	1:E:461:VAL:HG13	2.21	0.41
1:E:485:ASP:OD1	1:E:487:ARG:HB2	2.21	0.41
1:C:410:TRP:CD1	1:C:410:TRP:N	2.88	0.40
1:E:576:ARG:O	1:E:580:VAL:HG12	2.20	0.40
1:C:502:HIS:O	1:C:506:GLU:HG3	2.21	0.40
2:D:39:LEU:CB	2:D:43:MET:HE2	2.52	0.40
1:A:473:ILE:HD12	1:A:482:VAL:HG23	2.02	0.40
1:A:462:ASN:HD22	1:A:465:GLU:HG3	1.85	0.40
1:C:462:ASN:ND2	1:C:465:GLU:HG3	2.35	0.40
1:E:407:ASN:HD22	1:E:407:ASN:HA	1.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ARG:NH2	2:D:48:GLU:O[4_555]	2.17	0.03

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	221/232 (95%)	203 (92%)	15 (7%)	3 (1%)	9	19
1	C	222/232 (96%)	216 (97%)	5 (2%)	1 (0%)	24	46
1	E	221/232 (95%)	211 (96%)	7 (3%)	3 (1%)	9	19
2	B	79/94 (84%)	76 (96%)	2 (2%)	1 (1%)	9	21
2	D	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
2	F	79/94 (84%)	70 (89%)	8 (10%)	1 (1%)	9	21
All	All	902/978 (92%)	852 (94%)	41 (4%)	9 (1%)	12	28

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	49	ARG
1	A	476	LYS
1	C	476	LYS
1	E	499	GLN
1	A	521	ASN
2	B	92	GLY
1	A	526	LEU
1	E	498	GLY
1	E	526	LEU

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	207/214 (97%)	189 (91%)	18 (9%)	9	21
1	C	208/214 (97%)	194 (93%)	14 (7%)	15	33
1	E	207/214 (97%)	193 (93%)	14 (7%)	14	32
2	B	72/82 (88%)	65 (90%)	7 (10%)	8	17
2	D	73/82 (89%)	68 (93%)	5 (7%)	14	32
2	F	72/82 (88%)	65 (90%)	7 (10%)	8	17
All	All	839/888 (94%)	774 (92%)	65 (8%)	12	27

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	GLU
1	A	402	ILE
1	A	411	LEU
1	A	420	MET
1	A	448	SER
1	A	456	ARG
1	A	458	THR
1	A	461	VAL

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Mol	Chain	Res	Type
1	A	476	LYS
1	A	480	SER
1	A	515	GLU
1	A	524	LEU
1	A	532	HIS
1	A	559	ILE
1	A	571	GLN
1	A	574	LEU
1	A	577	LYS
1	A	580	VAL
2	B	37	THR
2	B	71	THR
2	B	80	GLU
2	B	82	THR
2	B	90	THR
2	B	93	VAL
2	B	95	GLU
1	C	366	LEU
1	C	370	GLU
1	C	371	ASP
1	C	396	ARG
1	C	402	ILE
1	C	411	LEU
1	C	437	VAL
1	C	461	VAL
1	C	494	LEU
1	C	497	MET
1	C	503	ARG
1	C	524	LEU
1	C	527	LEU
1	C	580	VAL
2	D	17	ILE
2	D	49	ARG
2	D	71	THR
2	D	80	GLU
2	D	95	GLU
1	E	407	ASN
1	E	416	ILE
1	E	437	VAL
1	E	455	LYS
1	E	461	VAL
1	E	476	LYS

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Mol	Chain	Res	Type
1	E	478	HIS
1	E	503	ARG
1	E	515	GLU
1	E	527	LEU
1	E	574	LEU
1	E	577	LYS
1	E	580	VAL
1	E	587	GLN
2	F	33	ILE
2	F	57	ILE
2	F	58	ARG
2	F	68	GLU
2	F	69	THR
2	F	80	GLU
2	F	95	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	HIS
1	A	385	GLN
1	A	403	GLN
1	A	407	ASN
1	A	430	GLN
1	A	462	ASN
1	A	510	GLN
1	A	521	ASN
1	A	525	ASN
2	B	18	ASN
2	B	50	GLN
2	B	56	GLN
2	B	64	GLN
2	B	88	GLN
1	C	403	GLN
1	C	407	ASN
1	C	409	HIS
1	C	452	GLN
1	C	462	ASN
1	C	466	GLN
1	C	502	HIS
1	C	510	GLN
1	C	521	ASN

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Mol	Chain	Res	Type
1	C	587	GLN
2	D	50	GLN
1	E	385	GLN
1	E	403	GLN
1	E	407	ASN
1	E	462	ASN
1	E	510	GLN
1	E	521	ASN
1	E	532	HIS
1	E	541	GLN
1	E	587	GLN
2	F	36	HIS
2	F	50	GLN
2	F	87	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	223/232 (96%)	-0.22	4 (1%) 67 63	16, 39, 76, 110	0
1	C	224/232 (96%)	-0.46	0 100 100	16, 36, 60, 77	0
1	E	223/232 (96%)	0.00	10 (4%) 38 32	21, 46, 86, 107	0
2	B	81/94 (86%)	-0.11	0 100 100	29, 46, 77, 95	0
2	D	82/94 (87%)	-0.21	2 (2%) 59 54	32, 44, 75, 92	0
2	F	81/94 (86%)	0.61	4 (4%) 35 29	41, 67, 85, 97	0
All	All	914/978 (93%)	-0.14	20 (2%) 62 57	16, 44, 79, 110	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	93	VAL	4.8
1	E	536	PRO	4.3
1	A	534	MET	3.9
1	E	476	LYS	3.7
2	F	92	GLY	3.7
2	D	93	VAL	3.1
1	A	533	SER	2.9
1	E	533	SER	2.9
1	E	537	HIS	2.9
1	E	532	HIS	2.7
1	E	475	ARG	2.7
2	F	94	PRO	2.7
1	E	543	LEU	2.7
1	A	535	LYS	2.6
2	F	95	GLU	2.3
1	E	477	VAL	2.2
2	D	94	PRO	2.2
1	A	476	LYS	2.1
1	E	408	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	539	ILE	2.1

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.