



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:59 AM UTC

PDB ID : 5XAM / pdb_00005xam
Title : Crystal structure of SecDF in I form at 4 Å resolution
Authors : Tsukazaki, T.; Tanaka, Y.; Furukwa, A.
Deposited on : 2017-03-14
Resolution : 4.00 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

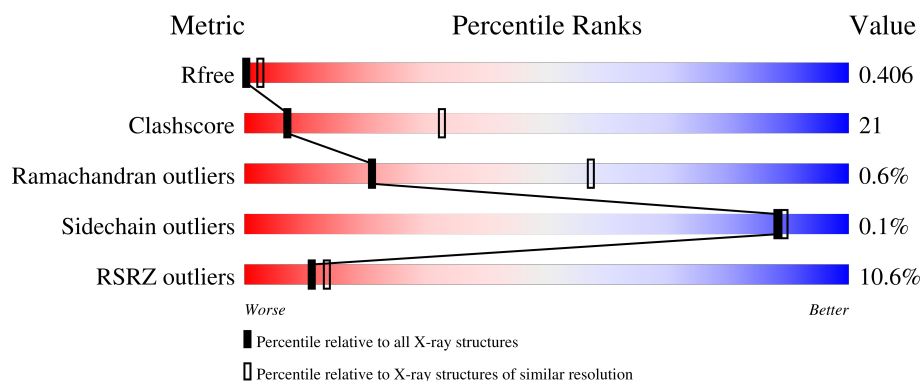
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	750	10% 63% 33% .
1	B	750	10% 54% 37% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9852 atoms, of which 0 are hydrogens and 0 are deuteriums.

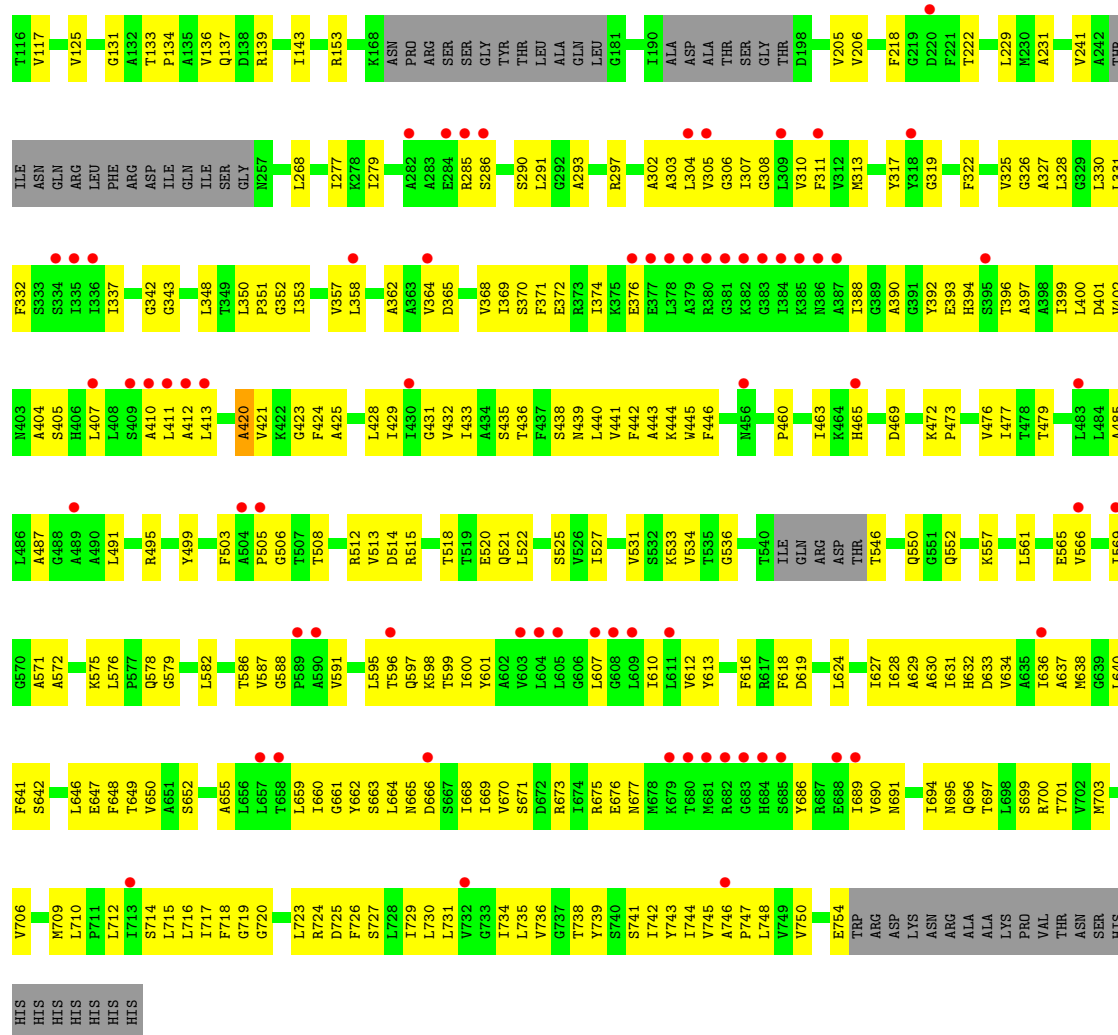
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein translocase subunit SecD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5000	3215	830	947	8			
1	B	684	Total	C	N	O	S	0	0	0
			4852	3140	801	900	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q9RTE3
A	769	HIS	-	expression tag	UNP Q9RTE3
A	770	HIS	-	expression tag	UNP Q9RTE3
A	771	HIS	-	expression tag	UNP Q9RTE3
A	772	HIS	-	expression tag	UNP Q9RTE3
A	773	HIS	-	expression tag	UNP Q9RTE3
A	774	HIS	-	expression tag	UNP Q9RTE3
A	775	HIS	-	expression tag	UNP Q9RTE3
A	776	HIS	-	expression tag	UNP Q9RTE3
B	27	MET	-	expression tag	UNP Q9RTE3
B	769	HIS	-	expression tag	UNP Q9RTE3
B	770	HIS	-	expression tag	UNP Q9RTE3
B	771	HIS	-	expression tag	UNP Q9RTE3
B	772	HIS	-	expression tag	UNP Q9RTE3
B	773	HIS	-	expression tag	UNP Q9RTE3
B	774	HIS	-	expression tag	UNP Q9RTE3
B	775	HIS	-	expression tag	UNP Q9RTE3
B	776	HIS	-	expression tag	UNP Q9RTE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.32Å 62.26Å 181.71Å 90.00° 101.71° 90.00°	Depositor
Resolution (Å)	47.98 – 4.00 47.98 – 4.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (47.98-4.00) 96.7 (47.98-4.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.333 , 0.402 0.336 , 0.406	Depositor DCC
R_{free} test set	1762 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å ²)	150.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 394.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å ²)	242.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.44% 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	0.17	1/5071 (0.0%)	0.39	0/6964
1	B	0.15	0/4926	0.40	0/6735
All	All	0.16	1/9997 (0.0%)	0.40	0/13699

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ARG	C-N	6.12	1.48	1.33

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	5000	0	4921	198	0
1	B	4852	0	4894	212	0
All	All	9852	0	9815	410	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 21.

All (410) 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:30:PRO:HG2	1:A:448:GLN:HG2	1.48	0.92
1:B:690:VAL:HG21	1:B:750:VAL:HG11	1.60	0.83
1:B:561:LEU:HB2	1:B:565:GLU:HB3	1.61	0.82
1:A:34:THR:HA	1:A:37:LEU:HB3	1.60	0.82
1:A:404:ALA:HA	1:A:407:LEU:HB2	1.62	0.80
1:B:438:SER:HA	1:B:442:PHE:HB3	1.62	0.80
1:B:531:VAL:HB	1:B:534:VAL:HG12	1.63	0.79
1:A:368:VAL:O	1:A:372:GLU:N	2.13	0.78
1:B:619:ASP:HB3	1:B:675:ARG:HH22	1.48	0.76
1:A:591:VAL:HA	1:A:594:GLU:HB2	1.68	0.75
1:B:618:PHE:HZ	1:B:668:ILE:HA	1.52	0.74
1:A:641:PHE:HE2	1:A:648:PHE:HB3	1.52	0.74
1:B:35:ALA:HB2	1:B:445:TRP:CH2	2.24	0.73
1:A:561:LEU:HB2	1:A:565:GLU:HG3	1.71	0.73
1:B:531:VAL:HG12	1:B:533:LYS:H	1.52	0.73
1:B:709:MET:HE1	1:B:731:LEU:HB2	1.71	0.73
1:B:137:GLN:NE2	1:B:286:SER:OG	2.22	0.72
1:B:741:SER:HA	1:B:745:VAL:HB	1.73	0.71
1:B:368:VAL:O	1:B:372:GLU:N	2.21	0.71
1:B:100:LYS:HG2	1:B:117:VAL:HG21	1.72	0.71
1:B:70:MET:HG3	1:B:342:GLY:HA3	1.72	0.70
1:A:205:VAL:HG12	1:A:206:VAL:H	1.56	0.70
1:A:641:PHE:CE2	1:A:648:PHE:HB3	2.26	0.70
1:B:399:ILE:HD11	1:B:439:ASN:HB3	1.71	0.70
1:A:662:TYR:O	1:A:665:ASN:ND2	2.24	0.69
1:B:472:LYS:HG3	1:B:473:PRO:HD3	1.74	0.69
1:B:712:LEU:HD12	1:B:731:LEU:HB3	1.74	0.69
1:A:673:ARG:NH2	1:A:693:ALA:O	2.26	0.68
1:A:513:VAL:HB	1:A:579:GLY:HA3	1.76	0.68
1:B:719:GLY:HA2	1:B:723:LEU:HD22	1.76	0.68
1:A:396:THR:O	1:A:400:LEU:N	2.16	0.68
1:A:618:PHE:HE1	1:A:668:ILE:HG12	1.59	0.67
1:A:491:LEU:HA	1:A:495:ARG:HB3	1.76	0.67
1:B:401:ASP:OD1	1:B:613:TYR:OH	2.13	0.67
1:B:313:MET:HE3	1:B:706:VAL:HG11	1.77	0.67
1:B:368:VAL:HA	1:B:371:PHE:HB3	1.75	0.67
1:A:402:VAL:O	1:A:406:HIS:ND1	2.29	0.66
1:B:134:PRO:HA	1:B:137:GLN:HB3	1.78	0.65
1:A:611:LEU:HA	1:A:614:VAL:HG12	1.79	0.65
1:B:720:GLY:H	1:B:723:LEU:HD13	1.62	0.64
1:B:231:ALA:HA	1:B:241:VAL:HG21	1.78	0.64
1:B:476:VAL:HA	1:B:479:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:ILE:HG23	1:A:748:LEU:HD22	1.80	0.64
1:A:186:THR:HG1	1:A:189:THR:HG1	1.44	0.63
1:A:604:LEU:O	1:A:608:GLY:N	2.29	0.63
1:A:561:LEU:HD13	1:A:565:GLU:HB2	1.80	0.63
1:B:96:LEU:HB2	1:B:125:VAL:HG21	1.81	0.62
1:B:319:GLY:HA2	1:B:460:PRO:HD2	1.81	0.62
1:B:628:ILE:O	1:B:632:HIS:N	2.28	0.62
1:B:374:ILE:HD12	1:B:388:ILE:HA	1.82	0.62
1:B:51:ARG:HH21	1:B:343:GLY:HA3	1.64	0.62
1:A:57:ASN:HD22	1:A:64:ASN:HB2	1.64	0.61
1:A:742:ILE:HG23	1:A:743:TYR:HD1	1.65	0.61
1:B:86:PRO:HB3	1:B:277:ILE:HG21	1.82	0.61
1:A:30:PRO:HG2	1:A:448:GLN:CG	2.27	0.61
1:B:630:ALA:HB1	1:B:660:ILE:HD12	1.82	0.61
1:B:428:LEU:O	1:B:432:VAL:HG12	2.00	0.61
1:A:618:PHE:CE1	1:A:668:ILE:HG12	2.35	0.60
1:A:403:ASN:O	1:A:407:LEU:N	2.35	0.60
1:B:527:ILE:HD12	1:B:536:GLY:HA2	1.83	0.60
1:A:666:ASP:OD1	1:A:741:SER:OG	2.14	0.59
1:A:735:LEU:O	1:A:739:TYR:HB3	2.01	0.59
1:A:664:LEU:O	1:A:668:ILE:HG13	2.02	0.59
1:A:413:LEU:HD23	1:A:657:LEU:HD11	1.85	0.59
1:B:513:VAL:HG11	1:B:576:LEU:HD23	1.83	0.59
1:A:45:SER:OG	1:A:335:ILE:O	2.21	0.59
1:B:691:ASN:O	1:B:695:ASN:ND2	2.36	0.59
1:B:506:GLY:N	1:B:587:VAL:HG11	2.18	0.59
1:A:513:VAL:HG21	1:A:576:LEU:HG	1.83	0.58
1:B:435:SER:OG	1:B:439:ASN:ND2	2.36	0.58
1:A:407:LEU:O	1:A:411:LEU:N	2.36	0.58
1:B:633:ASP:OD2	1:B:663:SER:OG	2.22	0.58
1:B:374:ILE:HG21	1:B:388:ILE:HG22	1.86	0.58
1:A:673:ARG:HH21	1:A:697:THR:HG23	1.69	0.57
1:B:325:VAL:HG22	1:B:446:PHE:HE2	1.70	0.57
1:B:72:LEU:HB2	1:B:77:LYS:HD3	1.86	0.57
1:B:404:ALA:HA	1:B:407:LEU:HB2	1.86	0.57
1:B:724:ARG:HA	1:B:727:SER:HB3	1.85	0.57
1:A:369:ILE:O	1:A:373:ARG:N	2.34	0.57
1:A:360:ILE:O	1:A:364:VAL:HG22	2.04	0.57
1:A:367:ASN:HA	1:A:439:ASN:OD1	2.03	0.56
1:A:610:ILE:O	1:A:614:VAL:N	2.26	0.56
1:B:508:THR:HG22	1:B:557:LYS:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ASP:HB3	1:B:578:GLN:HB2	1.88	0.56
1:A:418:THR:HG22	1:A:419:GLY:H	1.70	0.56
1:B:546:THR:HA	1:B:720:GLY:HA2	1.86	0.56
1:B:719:GLY:O	1:B:724:ARG:NH1	2.38	0.56
1:B:440:LEU:HG	1:B:441:VAL:HG13	1.87	0.56
1:B:505:PRO:HA	1:B:587:VAL:HG21	1.86	0.56
1:B:701:THR:HG21	1:B:742:ILE:HD11	1.88	0.56
1:B:424:PHE:O	1:B:428:LEU:HG	2.05	0.55
1:B:566:VAL:O	1:B:569:ILE:HG13	2.06	0.55
1:A:667:SER:HA	1:A:670:VAL:HG12	1.88	0.55
1:A:477:ILE:HG13	1:A:743:TYR:CD2	2.41	0.55
1:B:473:PRO:HB2	1:B:477:ILE:HG13	1.88	0.55
1:A:96:LEU:HB2	1:A:125:VAL:HG21	1.89	0.55
1:B:421:VAL:HG21	1:B:650:VAL:HB	1.89	0.55
1:A:736:VAL:HG22	1:A:740:SER:HB3	1.89	0.55
1:B:736:VAL:HA	1:B:739:TYR:CD1	2.42	0.55
1:B:76:LEU:HD11	1:B:350:LEU:HG	1.89	0.54
1:A:31:ASN:HD22	1:A:33:TRP:NE1	2.05	0.54
1:B:669:ILE:HG21	1:B:700:ARG:HB3	1.89	0.54
1:A:356:LEU:O	1:A:359:THR:OG1	2.21	0.54
1:A:371:PHE:O	1:A:375:LYS:NZ	2.40	0.54
1:A:408:LEU:HD11	1:A:609:LEU:HB3	1.90	0.54
1:A:340:ILE:HD13	1:A:430:ILE:HG13	1.89	0.54
1:A:673:ARG:NH2	1:A:697:THR:HG23	2.22	0.54
1:B:308:GLY:HA2	1:B:311:PHE:CE2	2.42	0.54
1:B:390:ALA:HA	1:B:393:GLU:HB2	1.89	0.54
1:B:677:ASN:HB3	1:B:689:ILE:HD11	1.89	0.54
1:B:694:ILE:CG2	1:B:742:ILE:HG23	2.38	0.54
1:A:31:ASN:OD1	1:A:31:ASN:N	2.38	0.54
1:A:609:LEU:O	1:A:613:TYR:N	2.41	0.54
1:B:715:LEU:HD23	1:B:727:SER:HB2	1.90	0.54
1:A:738:THR:O	1:A:742:ILE:HG22	2.08	0.53
1:A:57:ASN:N	1:A:57:ASN:OD1	2.41	0.53
1:B:322:PHE:HB3	1:B:371:PHE:CE2	2.43	0.53
1:A:593:LYS:HA	1:A:596:THR:HG22	1.89	0.53
1:B:627:ILE:O	1:B:631:ILE:HG12	2.09	0.53
1:A:477:ILE:HG21	1:A:743:TYR:HB3	1.91	0.53
1:A:503:PHE:HE1	1:A:650:VAL:HG22	1.74	0.53
1:B:720:GLY:N	1:B:723:LEU:HD13	2.23	0.53
1:A:666:ASP:HA	1:A:669:ILE:HB	1.89	0.53
1:B:51:ARG:HH11	1:B:53:TRP:HE1	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:HB3	1:B:425:ALA:HB2	1.90	0.53
1:A:513:VAL:HG13	1:A:514:ASP:H	1.73	0.53
1:A:502:ASP:C	1:A:595:LEU:HD11	2.34	0.52
1:A:577:PRO:O	1:A:578:GLN:HB2	2.09	0.52
1:A:614:VAL:O	1:A:618:PHE:HB2	2.09	0.52
1:A:491:LEU:O	1:A:642:SER:OG	2.23	0.52
1:B:697:THR:HA	1:B:700:ARG:HG3	1.90	0.52
1:A:502:ASP:HB3	1:A:595:LEU:HD13	1.91	0.52
1:B:357:VAL:HG11	1:B:715:LEU:HD22	1.90	0.52
1:B:513:VAL:HA	1:B:579:GLY:HA2	1.90	0.52
1:B:607:LEU:HA	1:B:610:ILE:HG12	1.89	0.52
1:B:624:LEU:HA	1:B:627:ILE:HB	1.89	0.52
1:A:477:ILE:HG13	1:A:743:TYR:HD2	1.74	0.52
1:A:598:LYS:HA	1:A:601:TYR:HD2	1.74	0.52
1:B:396:THR:HA	1:B:399:ILE:HG22	1.90	0.52
1:A:341:LEU:HD11	1:A:427:THR:HG22	1.91	0.52
1:B:86:PRO:HA	1:B:279:ILE:HG22	1.91	0.52
1:B:641:PHE:CD2	1:B:729:ILE:HD11	2.45	0.52
1:B:368:VAL:HG11	1:B:703:MET:HB3	1.92	0.52
1:A:609:LEU:HA	1:A:612:VAL:HB	1.92	0.52
1:A:637:ALA:HB1	1:A:656:LEU:HD22	1.91	0.52
1:A:507:THR:HG23	1:A:560:GLU:HA	1.92	0.52
1:A:513:VAL:HG11	1:A:576:LEU:HG	1.91	0.51
1:A:95:GLU:O	1:A:99:VAL:HG23	2.10	0.51
1:B:399:ILE:CD1	1:B:439:ASN:HB3	2.38	0.51
1:A:406:HIS:HE1	1:A:665:ASN:HB2	1.76	0.51
1:B:362:ALA:HA	1:B:365:ASP:HB3	1.93	0.51
1:B:400:LEU:O	1:B:404:ALA:N	2.41	0.51
1:B:512:ARG:NH2	1:B:550:GLN:HG2	2.26	0.51
1:A:117:VAL:HG13	1:A:127:VAL:HG22	1.92	0.51
1:B:463:ILE:HD11	1:B:465:HIS:HD2	1.75	0.51
1:B:557:LYS:NZ	1:B:647:GLU:OE1	2.43	0.51
1:A:359:THR:O	1:A:363:ALA:N	2.41	0.51
1:A:513:VAL:HG13	1:A:514:ASP:N	2.26	0.51
1:B:306:GLY:HA2	1:B:714:SER:HB3	1.93	0.51
1:B:670:VAL:HG11	1:B:746:ALA:HB2	1.92	0.50
1:B:304:LEU:O	1:B:308:GLY:N	2.44	0.50
1:B:655:ALA:HB2	1:B:726:PHE:HB3	1.93	0.50
1:B:739:TYR:O	1:B:743:TYR:HB2	2.12	0.50
1:B:515:ARG:HA	1:B:552:GLN:HG3	1.93	0.50
1:B:96:LEU:HA	1:B:99:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:VAL:O	1:B:368:VAL:HG23	2.11	0.50
1:B:673:ARG:HA	1:B:676:GLU:OE2	2.11	0.50
1:A:353:ILE:HD12	1:A:354:ALA:N	2.25	0.50
1:B:36:LEU:H	1:B:36:LEU:HD12	1.76	0.50
1:B:319:GLY:HA3	1:B:322:PHE:HB2	1.94	0.50
1:B:619:ASP:HB3	1:B:675:ARG:NH2	2.23	0.50
1:A:659:LEU:HD11	1:A:733:GLY:HA3	1.92	0.50
1:A:690:VAL:O	1:A:694:ILE:HG12	2.12	0.50
1:A:742:ILE:HG23	1:A:743:TYR:CD1	2.46	0.50
1:B:641:PHE:HZ	1:B:648:PHE:HA	1.76	0.50
1:A:746:ALA:HB3	1:A:747:PRO:HD3	1.93	0.50
1:A:638:MET:O	1:A:642:SER:N	2.45	0.50
1:A:752:PHE:O	1:A:756:ARG:N	2.36	0.50
1:B:330:LEU:HD12	1:B:331:LEU:N	2.27	0.50
1:B:438:SER:O	1:B:443:ALA:N	2.43	0.50
1:A:673:ARG:NH1	1:A:696:GLN:HB3	2.26	0.49
1:B:75:ASP:OD1	1:B:75:ASP:N	2.41	0.49
1:B:499:TYR:CB	1:B:648:PHE:HB2	2.42	0.49
1:B:597:GLN:HG2	1:B:601:TYR:CD2	2.47	0.49
1:A:709:MET:HE1	1:A:734:ILE:HB	1.94	0.49
1:A:736:VAL:HA	1:A:739:TYR:HD2	1.77	0.49
1:B:45:SER:O	1:B:49:ILE:HG22	2.12	0.49
1:B:469:ASP:HB3	1:B:472:LYS:HE3	1.94	0.49
1:B:518:THR:HG22	1:B:520:GLU:H	1.78	0.49
1:A:712:LEU:HD21	1:A:727:SER:O	2.13	0.49
1:B:307:ILE:HD11	1:B:330:LEU:HD13	1.93	0.49
1:B:410:ALA:HB1	1:B:429:ILE:HG12	1.95	0.49
1:B:302:ALA:HB1	1:B:715:LEU:HA	1.95	0.49
1:B:370:SER:O	1:B:374:ILE:HG12	2.12	0.49
1:A:595:LEU:HD12	1:A:596:THR:N	2.28	0.49
1:A:640:LEU:O	1:A:643:LEU:HG	2.13	0.48
1:A:732:VAL:O	1:A:736:VAL:HG12	2.13	0.48
1:A:35:ALA:HB2	1:A:445:TRP:CZ2	2.49	0.48
1:A:440:LEU:HD23	1:A:441:VAL:HG23	1.95	0.48
1:A:729:ILE:HD12	1:A:730:LEU:N	2.28	0.48
1:B:358:LEU:HD13	1:B:730:LEU:HD21	1.95	0.48
1:A:502:ASP:HB3	1:A:595:LEU:CD1	2.44	0.48
1:B:664:LEU:O	1:B:668:ILE:HG13	2.14	0.48
1:A:359:THR:HA	1:A:362:ALA:HB3	1.93	0.48
1:A:359:THR:HG23	1:A:428:LEU:HD23	1.96	0.48
1:B:51:ARG:O	1:B:55:HIS:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:O	1:A:49:ILE:HG13	2.14	0.48
1:A:186:THR:OG1	1:A:189:THR:OG1	2.17	0.48
1:B:308:GLY:HA2	1:B:311:PHE:CZ	2.49	0.48
1:B:322:PHE:HB3	1:B:371:PHE:HE2	1.79	0.48
1:A:439:ASN:O	1:A:443:ALA:HB3	2.14	0.48
1:A:633:ASP:OD2	1:A:737:GLY:HA2	2.14	0.48
1:B:34:THR:O	1:B:38:LEU:N	2.39	0.48
1:B:50:TRP:O	1:B:52:PRO:HD3	2.13	0.48
1:B:64:ASN:H	1:B:64:ASN:HD22	1.62	0.48
1:B:73:GLY:N	1:B:348:LEU:O	2.46	0.48
1:B:411:LEU:HD12	1:B:412:ALA:N	2.29	0.48
1:B:666:ASP:OD2	1:B:701:THR:HG23	2.14	0.48
1:A:570:GLY:O	1:A:574:GLY:N	2.45	0.48
1:A:608:GLY:O	1:A:611:LEU:HG	2.13	0.48
1:B:699:SER:O	1:B:703:MET:HG2	2.13	0.48
1:A:105:ASN:HA	1:A:108:ASN:HD22	1.78	0.47
1:A:310:VAL:HG13	1:A:314:LEU:HD12	1.96	0.47
1:A:332:PHE:O	1:A:336:ILE:HG13	2.14	0.47
1:B:485:ALA:HA	1:B:636:ILE:HG12	1.94	0.47
1:A:43:LEU:HD23	1:A:46:LEU:HD12	1.96	0.47
1:A:364:VAL:HG23	1:A:707:SER:HB2	1.95	0.47
1:B:512:ARG:HH22	1:B:550:GLN:H	1.60	0.47
1:A:712:LEU:CD2	1:A:731:LEU:HB2	2.44	0.47
1:B:522:LEU:HD13	1:B:576:LEU:HD22	1.95	0.47
1:A:744:ILE:O	1:A:748:LEU:HB2	2.14	0.47
1:B:432:VAL:O	1:B:436:THR:HG23	2.14	0.47
1:A:435:SER:O	1:A:438:SER:OG	2.32	0.47
1:B:376:GLU:OE2	1:B:696:GLN:NE2	2.47	0.47
1:B:746:ALA:HB3	1:B:747:PRO:HD3	1.96	0.47
1:A:150:LEU:HB3	1:A:187:GLY:HA2	1.96	0.47
1:A:62:LEU:HD11	1:A:68:GLN:O	2.14	0.47
1:B:410:ALA:HA	1:B:428:LEU:HD13	1.97	0.47
1:B:686:TYR:HE1	1:B:754:GLU:HB2	1.80	0.47
1:A:354:ALA:HA	1:A:357:VAL:HG22	1.97	0.47
1:A:406:HIS:HB3	1:A:432:VAL:HG11	1.95	0.47
1:B:513:VAL:HG12	1:B:514:ASP:OD1	2.15	0.47
1:B:586:THR:HG22	1:B:587:VAL:H	1.80	0.47
1:B:638:MET:O	1:B:642:SER:N	2.48	0.47
1:B:744:ILE:O	1:B:748:LEU:N	2.45	0.47
1:A:155:VAL:HG21	1:A:229:LEU:HD12	1.96	0.47
1:B:503:PHE:HB2	1:B:596:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:LEU:HD21	1:B:725:ASP:HB3	1.96	0.47
1:B:34:THR:HG23	1:B:445:TRP:CE3	2.50	0.47
1:B:717:ILE:HG13	1:B:718:PHE:CD2	2.50	0.47
1:A:364:VAL:O	1:A:368:VAL:N	2.48	0.46
1:B:205:VAL:HG12	1:B:206:VAL:H	1.79	0.46
1:B:487:ALA:O	1:B:491:LEU:HG	2.14	0.46
1:B:218:PHE:O	1:B:222:THR:OG1	2.28	0.46
1:B:352:GLY:HA2	1:B:423:GLY:C	2.40	0.46
1:B:317:TYR:HE2	1:B:703:MET:SD	2.38	0.46
1:B:697:THR:O	1:B:701:THR:N	2.48	0.46
1:A:712:LEU:HD21	1:A:731:LEU:HB2	1.97	0.46
1:B:491:LEU:HB3	1:B:495:ARG:HD2	1.97	0.46
1:A:191:ALA:HB1	1:A:209:LYS:O	2.15	0.46
1:A:324:LEU:HD11	1:A:328:LEU:HD12	1.97	0.46
1:B:332:PHE:HD2	1:B:438:SER:HB2	1.80	0.46
1:B:350:LEU:O	1:B:353:ILE:HG22	2.16	0.46
1:B:618:PHE:CE2	1:B:671:SER:HB3	2.51	0.46
1:A:233:VAL:HG22	1:A:238:ILE:HG12	1.97	0.46
1:A:392:TYR:O	1:A:396:THR:HG23	2.16	0.46
1:A:606:GLY:O	1:A:610:ILE:HB	2.16	0.46
1:A:660:ILE:O	1:A:664:LEU:N	2.39	0.46
1:B:291:LEU:H	1:B:582:LEU:HD21	1.80	0.46
1:B:337:ILE:HD11	1:B:431:GLY:HA2	1.98	0.46
1:B:624:LEU:HD12	1:B:627:ILE:HB	1.98	0.46
1:A:415:ASN:OD1	1:A:416:TYR:N	2.49	0.46
1:A:488:GLY:HA2	1:A:491:LEU:HB2	1.97	0.46
1:A:632:HIS:O	1:A:636:ILE:HG12	2.16	0.46
1:A:96:LEU:H	1:A:96:LEU:HD23	1.80	0.46
1:A:189:THR:OG1	1:A:189:THR:O	2.32	0.46
1:B:80:LEU:HB2	1:B:285:ARG:O	2.16	0.46
1:B:472:LYS:HG3	1:B:473:PRO:CD	2.44	0.46
1:A:233:VAL:HG22	1:A:238:ILE:HG23	1.98	0.46
1:A:665:ASN:CG	1:A:666:ASP:N	2.73	0.46
1:B:229:LEU:HD13	1:B:229:LEU:O	2.16	0.46
1:B:591:VAL:O	1:B:595:LEU:HB2	2.16	0.46
1:B:634:VAL:HA	1:B:637:ALA:HB3	1.97	0.46
1:A:337:ILE:HD11	1:A:431:GLY:HA2	1.98	0.45
1:B:405:SER:OG	1:B:661:GLY:O	2.23	0.45
1:A:619:ASP:HB2	1:A:622:MET:HB3	1.98	0.45
1:A:240:SER:OG	1:A:254:ILE:HD12	2.16	0.45
1:A:417:SER:OG	1:A:421:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:TYR:C	1:A:665:ASN:HD22	2.21	0.45
1:B:328:LEU:HD21	1:B:446:PHE:CD2	2.52	0.45
1:A:364:VAL:CG2	1:A:707:SER:HB2	2.46	0.45
1:A:401:ASP:OD1	1:A:668:ILE:HG21	2.17	0.45
1:B:133:THR:HB	1:B:136:VAL:HG23	1.98	0.45
1:B:326:GLY:O	1:B:330:LEU:N	2.48	0.45
1:A:501:VAL:O	1:A:587:VAL:HG21	2.16	0.45
1:B:293:ALA:O	1:B:297:ARG:HG2	2.17	0.45
1:B:433:ILE:O	1:B:436:THR:OG1	2.28	0.45
1:B:599:THR:OG1	1:B:600:ILE:N	2.50	0.45
1:B:734:ILE:O	1:B:738:THR:HG23	2.17	0.45
1:B:358:LEU:HD21	1:B:662:TYR:HE2	1.82	0.45
1:B:518:THR:HB	1:B:521:GLN:HB2	1.98	0.45
1:B:525:SER:OG	1:B:572:ALA:HB1	2.17	0.45
1:A:79:GLY:N	1:A:131:GLY:H	2.15	0.45
1:A:397:ALA:HA	1:A:400:LEU:HB3	1.99	0.45
1:A:656:LEU:HD23	1:A:729:ILE:HD13	1.99	0.45
1:A:492:VAL:O	1:A:496:GLY:HA2	2.16	0.44
1:A:699:SER:O	1:A:703:MET:HG2	2.17	0.44
1:B:139:ARG:O	1:B:143:ILE:HG12	2.17	0.44
1:A:515:ARG:HA	1:A:552:GLN:N	2.32	0.44
1:B:392:TYR:O	1:B:396:THR:N	2.50	0.44
1:A:721:PRO:O	1:A:724:ARG:N	2.51	0.44
1:A:392:TYR:HA	1:A:395:SER:HB3	1.99	0.44
1:B:472:LYS:CG	1:B:473:PRO:HD3	2.45	0.44
1:B:634:VAL:HG12	1:B:659:LEU:HD23	1.98	0.44
1:A:64:ASN:OD1	1:A:65:ASP:N	2.48	0.44
1:B:305:VAL:HA	1:B:308:GLY:HA3	1.99	0.44
1:B:110:LEU:HB3	1:B:112:VAL:HG23	1.98	0.44
1:A:328:LEU:HB3	1:A:446:PHE:CZ	2.53	0.44
1:B:735:LEU:O	1:B:738:THR:OG1	2.31	0.44
1:A:310:VAL:HG22	1:A:710:LEU:HD12	2.00	0.43
1:A:593:LYS:O	1:A:597:GLN:HG3	2.18	0.43
1:A:715:LEU:HD11	1:A:723:LEU:HG	2.00	0.43
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.74	0.43
1:B:303:ALA:O	1:B:307:ILE:N	2.48	0.43
1:B:669:ILE:H	1:B:669:ILE:HG13	1.55	0.43
1:B:99:VAL:HA	1:B:102:VAL:HG22	2.01	0.43
1:B:310:VAL:HG22	1:B:710:LEU:HB2	2.00	0.43
1:B:332:PHE:CD2	1:B:438:SER:HB2	2.53	0.43
1:B:597:GLN:O	1:B:601:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ALA:HA	1:B:632:HIS:HB3	2.01	0.43
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.92	0.43
1:A:403:ASN:OD1	1:A:404:ALA:N	2.51	0.43
1:A:266:LEU:O	1:A:270:LEU:HG	2.17	0.43
1:A:618:PHE:CD2	1:A:623:GLY:HA2	2.53	0.43
1:B:290:SER:HB2	1:B:582:LEU:HD21	2.00	0.43
1:A:402:VAL:HG23	1:A:669:ILE:HD11	2.00	0.43
1:A:408:LEU:HD13	1:A:613:TYR:HB2	2.01	0.43
1:B:38:LEU:HD13	1:B:445:TRP:CD1	2.53	0.43
1:A:79:GLY:O	1:A:287:ILE:HD12	2.18	0.43
1:A:107:ILE:HD11	1:A:115:PRO:HG3	2.01	0.43
1:B:665:ASN:HA	1:B:668:ILE:HD12	1.99	0.43
1:A:117:VAL:HG22	1:A:127:VAL:HG13	2.00	0.43
1:A:425:ALA:O	1:A:429:ILE:HG13	2.19	0.42
1:B:369:ILE:HG12	1:B:402:VAL:HG21	2.01	0.42
1:B:744:ILE:C	1:B:747:PRO:HD2	2.43	0.42
1:A:388:ILE:HG13	1:A:389:GLY:N	2.35	0.42
1:A:400:LEU:HA	1:A:403:ASN:HD21	1.84	0.42
1:A:403:ASN:HB3	1:A:436:THR:HG21	2.02	0.42
1:A:545:THR:HG22	1:A:553:ASN:N	2.35	0.42
1:B:595:LEU:HD12	1:B:598:LYS:HD3	2.01	0.42
1:B:716:LEU:HD23	1:B:724:ARG:HG2	2.01	0.42
1:A:162:ASP:O	1:A:166:ARG:N	2.53	0.42
1:A:725:ASP:O	1:A:729:ILE:HG13	2.19	0.42
1:B:641:PHE:CE2	1:B:646:LEU:HD23	2.54	0.42
1:A:49:ILE:HD11	1:A:335:ILE:O	2.19	0.42
1:A:572:ALA:HA	1:A:575:LYS:NZ	2.34	0.42
1:B:64:ASN:H	1:B:64:ASN:ND2	2.17	0.42
1:A:119:VAL:HA	1:A:125:VAL:HA	2.02	0.42
1:B:34:THR:HG23	1:B:445:TRP:HE3	1.84	0.42
1:B:441:VAL:O	1:B:445:TRP:N	2.52	0.42
1:B:48:TYR:HA	1:B:51:ARG:HD3	2.01	0.42
1:A:71:THR:HB	1:A:346:ALA:O	2.19	0.42
1:A:359:THR:HG21	1:A:431:GLY:HA3	2.02	0.42
1:A:375:LYS:O	1:A:378:LEU:HG	2.19	0.42
1:A:713:ILE:O	1:A:717:ILE:HG13	2.19	0.42
1:A:422:LYS:O	1:A:425:ALA:HB3	2.20	0.42
1:A:503:PHE:CE1	1:A:650:VAL:HG22	2.54	0.42
1:A:712:LEU:HA	1:A:715:LEU:HB3	2.01	0.42
1:A:721:PRO:O	1:A:724:ARG:HG2	2.20	0.42
1:B:351:PRO:HG3	1:B:420:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:VAL:O	1:B:616:PHE:N	2.50	0.42
1:A:104:GLU:HG2	1:A:117:VAL:HG21	2.02	0.41
1:B:561:LEU:HB2	1:B:565:GLU:CB	2.43	0.41
1:A:78:GLY:C	1:A:132:ALA:H	2.27	0.41
1:A:443:ALA:HA	1:A:446:PHE:CD2	2.55	0.41
1:A:662:TYR:CA	1:A:665:ASN:HD22	2.33	0.41
1:B:49:ILE:HD12	1:B:70:MET:HE2	2.02	0.41
1:B:629:ALA:HB2	1:B:745:VAL:HG21	2.01	0.41
1:B:649:THR:O	1:B:652:SER:HB2	2.20	0.41
1:A:191:ALA:HB1	1:A:210:THR:HA	2.02	0.41
1:A:518:THR:HA	1:A:522:LEU:HD12	2.01	0.41
1:A:618:PHE:HE2	1:A:622:MET:HE3	1.85	0.41
1:A:730:LEU:HD12	1:A:730:LEU:HA	1.95	0.41
1:B:641:PHE:HD2	1:B:729:ILE:HD11	1.83	0.41
1:A:375:LYS:HA	1:A:375:LYS:HD3	1.86	0.41
1:B:327:ALA:O	1:B:331:LEU:HB2	2.20	0.41
1:B:390:ALA:O	1:B:394:HIS:N	2.43	0.41
1:B:397:ALA:O	1:B:401:ASP:N	2.54	0.41
1:B:231:ALA:HA	1:B:241:VAL:HG11	2.03	0.41
1:A:328:LEU:HD13	1:A:446:PHE:CD1	2.56	0.41
1:B:370:SER:HB3	1:B:399:ILE:HD12	2.02	0.41
1:B:571:ALA:O	1:B:575:LYS:HD3	2.21	0.41
1:A:472:LYS:HB2	1:A:473:PRO:HD3	2.02	0.41
1:B:420:ALA:O	1:B:423:GLY:N	2.43	0.41
1:B:441:VAL:HA	1:B:444:LYS:HB3	2.03	0.41
1:A:79:GLY:HA3	1:A:130:PRO:HA	2.03	0.41
1:A:712:LEU:HD11	1:A:730:LEU:HB3	2.03	0.41
1:B:79:GLY:HA2	1:B:131:GLY:HA2	2.02	0.41
1:B:636:ILE:HG22	1:B:640:LEU:HD13	2.03	0.40
1:A:34:THR:HG23	1:A:37:LEU:HD23	2.03	0.40
1:A:73:GLY:HA2	1:A:348:LEU:O	2.21	0.40
1:B:631:ILE:HA	1:B:634:VAL:HG22	2.03	0.40
1:A:110:LEU:HD22	1:A:112:VAL:HG22	2.03	0.40
1:A:326:GLY:O	1:A:330:LEU:HD13	2.22	0.40
1:A:527:ILE:HG21	1:A:536:GLY:HA2	2.03	0.40
1:A:697:THR:O	1:A:701:THR:OG1	2.28	0.40
1:B:495:ARG:CZ	1:B:642:SER:HB3	2.52	0.40
1:B:587:VAL:HG22	1:B:588:GLY:H	1.85	0.40
1:A:646:LEU:HD12	1:A:646:LEU:HA	1.93	0.40
1:A:488:GLY:O	1:A:492:VAL:N	2.55	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	721/750 (96%)	656 (91%)	59 (8%)	6 (1%)	16	52
1	B	672/750 (90%)	622 (93%)	47 (7%)	3 (0%)	30	65
All	All	1393/1500 (93%)	1278 (92%)	106 (8%)	9 (1%)	21	57

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLN
1	A	721	PRO
1	B	51	ARG
1	A	446	PHE
1	B	420	ALA
1	A	276	PRO
1	B	153	ARG
1	A	460	PRO
1	A	455	PRO

5.3.2 Protein sidechains [i](#)

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	481/603 (80%)	480 (100%)	1 (0%)	87	87
1	B	484/603 (80%)	484 (100%)	0	100	100
All	All	965/1206 (80%)	964 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	57	ASN
1	A	66	GLN
1	A	108	ASN
1	A	367	ASN
1	A	677	ASN
1	B	31	ASN
1	B	137	GLN
1	B	225	ASN
1	B	465	HIS

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 ⓘ

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	727/750 (96%)	0.70	75 (10%) 12 14	93, 244, 354, 420	0
1	B	684/750 (91%)	0.68	74 (10%) 11 13	75, 237, 385, 441	0
All	All	1411/1500 (94%)	0.69	149 (10%) 11 13	75, 241, 366, 441	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	LYS	17.4
1	A	382	LYS	16.3
1	B	379	ALA	15.5
1	B	684	HIS	14.1
1	A	381	GLY	12.0
1	B	381	GLY	11.8
1	A	681	MET	11.4
1	A	680	THR	10.9
1	A	379	ALA	10.9
1	A	380	ARG	10.5
1	A	688	GLU	9.8
1	B	683	GLY	8.6
1	B	688	GLU	8.1
1	B	380	ARG	7.6
1	A	412	ALA	7.5
1	B	384	ILE	7.3
1	A	604	LEU	7.3
1	B	377	GLU	7.2
1	B	680	THR	7.1
1	A	377	GLU	7.1
1	A	607	LEU	6.9
1	A	684	HIS	6.9
1	A	603	VAL	6.8
1	A	685	SER	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	465	HIS	6.3
1	B	309	LEU	6.3
1	B	685	SER	6.1
1	B	386	ASN	6.0
1	B	681	MET	5.9
1	A	679	LYS	5.9
1	B	411	LEU	5.8
1	A	411	LEU	5.7
1	A	689	ILE	5.4
1	B	682	ARG	5.4
1	B	383	GLY	5.4
1	B	658	THR	5.3
1	A	602	ALA	5.3
1	A	413	LEU	5.0
1	B	358	LEU	4.9
1	A	41	THR	4.9
1	B	689	ILE	4.9
1	A	385	LYS	4.8
1	A	383	GLY	4.7
1	A	605	LEU	4.7
1	B	387	ALA	4.7
1	B	285	ARG	4.4
1	A	660	ILE	4.3
1	A	692	ALA	4.3
1	B	336	ILE	4.2
1	A	486	LEU	4.1
1	B	605	LEU	4.1
1	B	410	ALA	4.1
1	A	386	ASN	4.1
1	B	378	LEU	4.0
1	A	465	HIS	4.0
1	B	609	LEU	4.0
1	A	376	GLU	3.8
1	B	284	GLU	3.8
1	A	677	ASN	3.8
1	A	45	SER	3.7
1	B	409	SER	3.7
1	B	589	PRO	3.6
1	A	634	VAL	3.6
1	A	691	ASN	3.5
1	B	85	ALA	3.4
1	A	485	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	656	LEU	3.4
1	A	687	ARG	3.3
1	B	483	LEU	3.2
1	B	376	GLU	3.2
1	B	504	ALA	3.2
1	B	304	LEU	3.2
1	A	429	ILE	3.1
1	A	682	ARG	3.1
1	B	412	ALA	3.1
1	A	683	GLY	3.1
1	A	608	GLY	3.1
1	B	430	ILE	3.1
1	A	146	GLN	3.0
1	A	636	ILE	3.0
1	A	631	ILE	3.0
1	A	653	VAL	2.9
1	B	334	SER	2.9
1	B	713	ILE	2.9
1	A	615	GLY	2.9
1	A	378	LEU	2.8
1	A	606	GLY	2.8
1	B	407	LEU	2.8
1	A	336	ILE	2.8
1	B	115	PRO	2.8
1	A	466	THR	2.7
1	A	409	SER	2.7
1	B	45	SER	2.7
1	A	484	LEU	2.7
1	A	704	THR	2.6
1	A	148	ALA	2.6
1	B	305	VAL	2.6
1	A	415	ASN	2.6
1	A	44	GLY	2.6
1	B	608	GLY	2.6
1	A	284	GLU	2.6
1	A	334	SER	2.6
1	A	107	ILE	2.6
1	A	617	ARG	2.6
1	B	84	LEU	2.5
1	B	364	VAL	2.5
1	A	325	VAL	2.5
1	A	410	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	43	LEU	2.5
1	B	636	ILE	2.5
1	A	147	THR	2.5
1	B	413	LEU	2.4
1	B	657	LEU	2.4
1	B	282	ALA	2.4
1	A	635	ALA	2.4
1	B	611	LEU	2.4
1	B	318	TYR	2.4
1	A	144	ILE	2.4
1	B	732	VAL	2.4
1	A	658	THR	2.4
1	B	82	ILE	2.3
1	B	335	ILE	2.3
1	B	590	ALA	2.3
1	B	311	PHE	2.3
1	A	407	LEU	2.3
1	B	505	PRO	2.3
1	B	385	LYS	2.3
1	B	456	ASN	2.2
1	B	607	LEU	2.2
1	B	220	ASP	2.2
1	A	353	ILE	2.2
1	B	489	ALA	2.2
1	A	600	ILE	2.2
1	B	666	ASP	2.1
1	A	266	LEU	2.1
1	B	604	LEU	2.1
1	B	566	VAL	2.1
1	B	286	SER	2.1
1	A	397	ALA	2.1
1	A	430	ILE	2.1
1	B	569	ILE	2.1
1	B	395	SER	2.1
1	A	275	LEU	2.0
1	B	679	LYS	2.0
1	A	191	ALA	2.0
1	B	746	ALA	2.0
1	B	603	VAL	2.0
1	A	678	MET	2.0
1	B	596	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.