



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:55 PM UTC

PDB ID : 5JXB / pdb_00005jxb
Title : PSD-95 extended PDZ3 in complex with SynGAP PBM
Authors : Shang, Y.; Zhang, M.
Deposited on : 2016-05-13
Resolution : 2.90 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

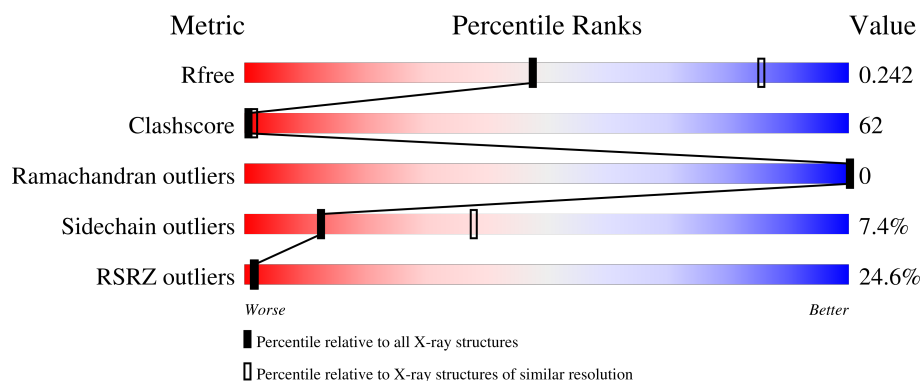
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	123	28% 34% 56% 5% 5%
1	C	123	19% 34% 53% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1781 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 Disks large homolog 4, SynGAP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			885	559	160	165	1			
1	C	119	Total	C	N	O	S	0	0	0
			892	562	162	167	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	GLU	-	expression tag	UNP P78352
A	305	PHE	-	expression tag	UNP P78352
A	411	GLY	-	linker	UNP P78352
A	412	SER	-	linker	UNP P78352
A	413	GLY	-	linker	UNP P78352
A	414	SER	-	linker	UNP P78352
C	304	GLU	-	expression tag	UNP P78352
C	305	PHE	-	expression tag	UNP P78352
C	411	GLY	-	linker	UNP P78352
C	412	SER	-	linker	UNP P78352
C	413	GLY	-	linker	UNP P78352
C	414	SER	-	linker	UNP P78352

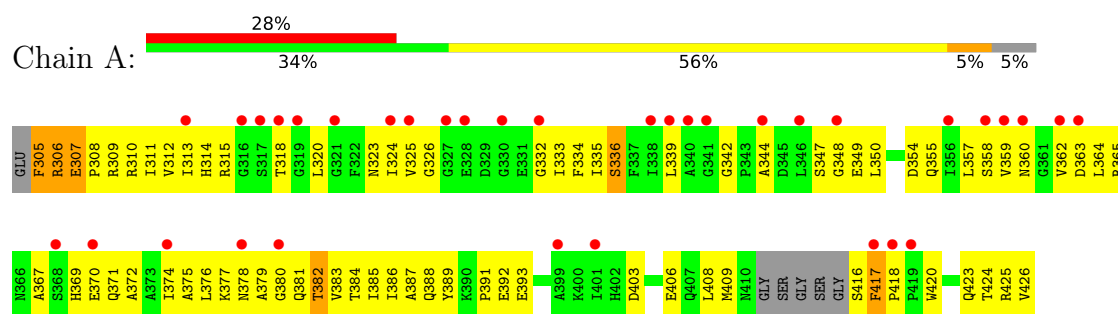
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	C	3	Total	O	0	0
			3	3		

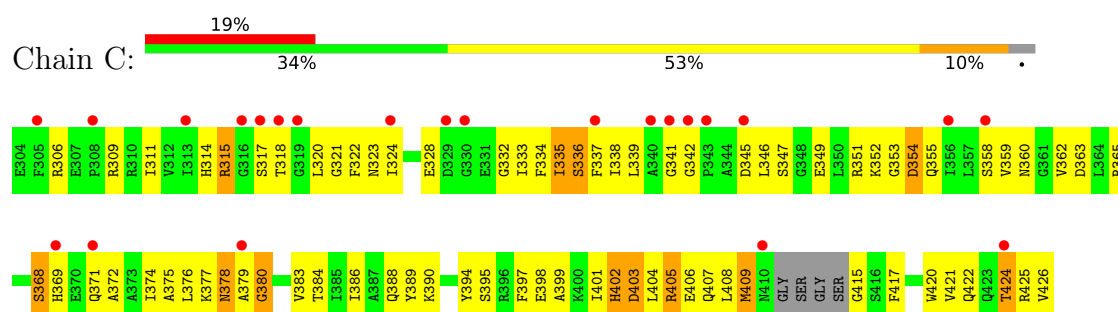
3 Residue-property plots [i](#)

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: Disks large homolog 4,SynGAP



• Molecule 1: Disks large homolog 4,SynGAP



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	70.29Å 71.09Å 115.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 2.90 45.89 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.89-2.90) 94.0 (45.89-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.40 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.241 , 0.287 0.236 , 0.242	Depositor DCC
R_{free} test set	370 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.871	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 174.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.380 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	1781	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% 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	0.63	1/901 (0.1%)	0.98	2/1216 (0.2%)
1	C	0.86	2/908 (0.2%)	1.21	13/1226 (1.1%)
All	All	0.75	3/1809 (0.2%)	1.10	15/2442 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	335	ILE	CG1-CD1	-8.51	1.18	1.51
1	C	405	ARG	CZ-NH2	-7.07	1.24	1.33
1	A	382	THR	CB-CG2	-5.36	1.34	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	405	ARG	CG-CD-NE	9.90	133.79	112.00
1	C	320	LEU	CA-CB-CG	8.08	144.59	116.30
1	C	409	MET	CG-SD-CE	-8.00	83.31	100.90
1	C	378	ASN	N-CA-C	7.42	119.37	111.28
1	C	403	ASP	CA-C-N	-7.32	108.77	121.66
1	C	403	ASP	C-N-CA	-7.32	108.77	121.66
1	C	380	GLY	CA-C-N	6.03	128.65	120.44
1	C	380	GLY	C-N-CA	6.03	128.65	120.44
1	A	382	THR	CA-CB-CG2	-6.03	100.25	110.50
1	C	335	ILE	CA-CB-CG1	-6.00	100.20	110.40
1	C	318	THR	N-CA-C	5.57	117.35	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	MET	CA-CB-CG	-5.43	103.25	114.10
1	A	307	GLU	N-CA-C	-5.28	103.03	110.31
1	C	402	HIS	CA-C-N	-5.18	112.06	120.72
1	C	402	HIS	C-N-CA	-5.18	112.06	120.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	354	ASP	Peptide
1	C	380	GLY	Peptide

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	885	0	856	99	0
1	C	892	0	853	127	0
2	A	1	0	0	0	0
2	C	3	0	0	3	0
All	All	1781	0	1709	217	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 62.

All (217) 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:351:ARG:HH12	1:C:354:ASP:CA	1.43	1.29
1:C:351:ARG:HH22	1:C:354:ASP:N	1.32	1.25
1:C:315:ARG:NH1	1:C:377:LYS:O	1.73	1.22
1:C:351:ARG:NH1	1:C:354:ASP:HA	1.58	1.16
1:C:374:ILE:O	1:C:378:ASN:N	1.82	1.13
1:C:402:HIS:O	1:C:405:ARG:HD2	1.51	1.11
1:C:351:ARG:CZ	1:C:354:ASP:HB3	1.82	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ARG:NH1	1:C:354:ASP:CA	2.13	1.07
1:C:351:ARG:NH1	1:C:354:ASP:HB3	1.69	1.07
1:A:379:ALA:HB1	1:A:383:VAL:HG21	1.33	1.06
1:C:405:ARG:HD3	1:C:406:GLU:H	1.16	1.03
1:C:323:ASN:HB3	1:C:425:ARG:HA	1.38	1.03
1:C:351:ARG:NH1	1:C:354:ASP:CB	2.22	1.02
1:C:323:ASN:CB	1:C:424:THR:O	2.08	1.00
1:C:323:ASN:HB2	1:C:424:THR:O	1.61	0.98
1:C:405:ARG:HD3	1:C:406:GLU:N	1.79	0.97
1:C:351:ARG:NH2	1:C:354:ASP:N	2.13	0.95
1:A:369:HIS:HE2	1:A:424:THR:HG1	1.10	0.94
1:C:335:ILE:HD11	1:C:352:LYS:HA	1.46	0.94
1:C:351:ARG:HH22	1:C:354:ASP:H	1.09	0.93
1:C:405:ARG:NH1	1:C:406:GLU:OE1	2.02	0.93
1:C:323:ASN:HD22	1:C:425:ARG:HG2	1.33	0.92
1:A:381:GLN:HG2	1:A:382:THR:H	1.35	0.91
1:A:314:HIS:CG	1:A:382:THR:HG21	2.09	0.88
1:C:351:ARG:HH12	1:C:354:ASP:HA	0.73	0.88
1:A:309:ARG:NH1	1:A:354:ASP:OD1	2.07	0.86
1:C:322:PHE:HB3	1:C:338:ILE:HG22	1.59	0.85
1:C:351:ARG:CZ	1:C:354:ASP:CB	2.55	0.84
1:A:344:ALA:O	1:A:348:GLY:N	2.12	0.83
1:A:376:LEU:HA	1:A:379:ALA:HB2	1.58	0.83
1:A:314:HIS:CD2	1:A:382:THR:HG21	2.15	0.81
1:C:402:HIS:O	1:C:405:ARG:CD	2.29	0.79
1:C:355:GLN:HE21	1:C:390:LYS:HE3	1.46	0.78
1:C:405:ARG:CZ	1:C:406:GLU:CD	2.57	0.77
1:A:309:ARG:NH2	1:A:349:GLU:O	2.18	0.77
1:A:381:GLN:O	1:A:382:THR:HG23	1.85	0.76
1:C:415:GLY:N	2:C:502:HOH:O	2.18	0.76
1:A:381:GLN:CG	1:A:382:THR:H	2.00	0.73
1:C:351:ARG:NH1	1:C:389:TYR:HA	2.03	0.73
1:A:416:SER:OG	1:A:417:PHE:N	2.22	0.71
1:A:310:ARG:NH1	1:C:328:GLU:OE2	2.24	0.70
1:C:379:ALA:HB3	1:C:383:VAL:HG11	1.72	0.70
1:C:405:ARG:NH1	1:C:406:GLU:CD	2.48	0.70
1:A:379:ALA:HB1	1:A:383:VAL:CG2	2.16	0.69
1:A:381:GLN:HG2	1:A:382:THR:N	2.07	0.69
1:C:405:ARG:NE	1:C:406:GLU:HG3	2.09	0.68
1:A:314:HIS:CE1	1:A:382:THR:HG21	2.29	0.67
1:C:323:ASN:HB3	1:C:424:THR:O	1.90	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PHE:CZ	1:C:339:LEU:HG	2.29	0.67
1:A:315:ARG:HH21	1:A:380:GLY:H	1.40	0.67
1:A:358:SER:HB2	1:A:386:ILE:HG12	1.77	0.67
1:C:351:ARG:CZ	1:C:354:ASP:CA	2.72	0.67
1:A:311:ILE:HB	1:A:385:ILE:HD11	1.78	0.66
1:C:376:LEU:HD23	1:C:426:VAL:HG21	1.77	0.66
1:A:305:PHE:CZ	1:A:392:GLU:OE1	2.48	0.66
1:A:347:SER:HB2	1:A:349:GLU:OE1	1.97	0.65
1:C:405:ARG:CD	1:C:406:GLU:HG3	2.25	0.65
1:A:357:LEU:N	1:A:357:LEU:HD12	2.11	0.65
1:A:364:LEU:HA	1:A:367:ALA:HB2	1.80	0.63
1:C:351:ARG:H	1:C:351:ARG:HD3	1.64	0.62
1:C:306:ARG:O	1:C:388:GLN:NE2	2.32	0.62
1:A:315:ARG:NH2	1:A:377:LYS:O	2.32	0.62
1:C:351:ARG:NH2	1:C:354:ASP:H	1.86	0.62
1:A:307:GLU:HA	1:C:409:MET:CE	2.30	0.62
1:C:334:PHE:HA	1:C:354:ASP:O	2.00	0.62
1:C:323:ASN:HA	1:C:426:VAL:HG22	1.80	0.61
1:A:359:VAL:O	1:A:362:VAL:HG12	2.02	0.60
1:A:369:HIS:CD2	1:A:424:THR:HG1	2.19	0.60
1:A:314:HIS:ND1	1:A:382:THR:HG21	2.17	0.60
1:A:306:ARG:HD3	1:A:389:TYR:O	2.02	0.60
1:A:389:TYR:OH	1:A:391:PRO:HB3	2.00	0.60
1:A:349:GLU:OE1	1:A:349:GLU:N	2.33	0.59
1:A:403:ASP:HA	1:A:406:GLU:HG2	1.85	0.59
1:C:358:SER:OG	2:C:501:HOH:O	2.16	0.59
1:A:369:HIS:NE2	1:A:424:THR:OG1	2.13	0.59
1:C:351:ARG:CZ	1:C:389:TYR:CD1	2.85	0.59
1:A:324:ILE:HD12	1:A:334:PHE:O	2.02	0.59
1:C:405:ARG:HH21	1:C:406:GLU:H	1.50	0.58
1:A:357:LEU:HB2	1:A:386:ILE:HG13	1.84	0.58
1:A:311:ILE:HD11	1:A:349:GLU:HB3	1.85	0.58
1:C:355:GLN:NE2	1:C:390:LYS:HE3	2.17	0.58
1:A:375:ALA:O	1:A:379:ALA:N	2.37	0.58
1:A:315:ARG:HH21	1:A:380:GLY:N	2.02	0.58
1:C:335:ILE:CD1	1:C:351:ARG:O	2.53	0.57
1:A:307:GLU:HA	1:C:409:MET:HE3	1.87	0.57
1:C:363:ASP:OD1	1:C:365:ARG:HD3	2.05	0.56
1:C:405:ARG:CZ	1:C:406:GLU:CG	2.83	0.56
1:C:374:ILE:O	1:C:378:ASN:CB	2.54	0.56
1:C:322:PHE:HE1	1:C:324:ILE:HG23	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:HIS:O	1:C:405:ARG:NE	2.38	0.56
1:C:401:ILE:HA	1:C:404:LEU:HD23	1.87	0.56
1:A:408:LEU:HD12	1:A:409:MET:HG2	1.87	0.55
1:C:368:SER:HB3	1:C:371:GLN:NE2	2.22	0.55
1:C:341:GLY:N	1:C:345:ASP:OD2	2.28	0.55
1:A:305:PHE:HZ	1:A:392:GLU:OE1	1.86	0.54
1:C:359:VAL:HA	1:C:384:THR:O	2.07	0.54
1:A:320:LEU:HD13	1:A:426:VAL:HG22	1.87	0.54
1:C:337:PHE:HE2	1:C:339:LEU:HA	1.73	0.54
1:C:335:ILE:HG23	1:C:354:ASP:OD1	2.08	0.54
1:C:405:ARG:CZ	1:C:406:GLU:OE1	2.50	0.53
1:A:324:ILE:HG22	1:A:424:THR:HB	1.91	0.53
1:A:311:ILE:O	1:A:385:ILE:HG13	2.09	0.53
1:C:337:PHE:HE1	1:C:425:ARG:HE	1.57	0.53
1:A:380:GLY:HA3	1:A:381:GLN:OE1	2.09	0.52
1:C:333:ILE:HG12	1:C:372:ALA:HB2	1.92	0.52
1:C:311:ILE:HD12	1:C:349:GLU:HB3	1.92	0.52
1:C:337:PHE:HZ	1:C:339:LEU:HG	1.74	0.52
1:C:376:LEU:CD2	1:C:426:VAL:HG21	2.38	0.52
1:A:314:HIS:HA	1:A:382:THR:HG22	1.92	0.52
1:A:315:ARG:NE	1:A:380:GLY:O	2.32	0.52
1:C:351:ARG:NH2	1:C:354:ASP:CA	2.72	0.52
1:C:321:GLY:O	1:C:339:LEU:N	2.44	0.51
1:A:381:GLN:C	1:A:382:THR:HG23	2.33	0.51
1:A:354:ASP:HB3	1:A:387:ALA:HB1	1.92	0.51
1:A:374:ILE:O	1:A:378:ASN:HB3	2.10	0.51
1:C:403:ASP:O	1:C:407:GLN:HG3	2.11	0.51
1:A:314:HIS:CG	1:A:382:THR:CG2	2.89	0.51
1:A:359:VAL:HG22	1:A:383:VAL:CG2	2.41	0.51
1:C:395:SER:HA	1:C:398:GLU:HG2	1.93	0.51
1:A:342:GLY:C	1:A:344:ALA:H	2.19	0.50
1:A:360:ASN:OD1	1:A:383:VAL:HA	2.11	0.50
1:C:374:ILE:O	1:C:378:ASN:CA	2.58	0.50
1:A:325:VAL:HG13	1:A:336:SER:OG	2.11	0.50
1:A:314:HIS:CD2	1:A:382:THR:CG2	2.89	0.50
1:C:336:SER:HA	1:C:394:TYR:OH	2.12	0.49
1:C:360:ASN:ND2	1:C:384:THR:H	2.10	0.49
1:C:337:PHE:CE2	1:C:339:LEU:HA	2.47	0.49
1:C:342:GLY:O	1:C:346:LEU:N	2.20	0.49
1:C:394:TYR:O	1:C:397:PHE:HB3	2.12	0.49
1:C:374:ILE:HG13	1:C:375:ALA:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:HIS:CE1	1:C:405:ARG:HH11	2.30	0.49
1:C:338:ILE:O	1:C:338:ILE:HD12	2.12	0.49
1:A:392:GLU:HG3	1:A:393:GLU:OE1	2.14	0.48
1:C:351:ARG:HH22	1:C:353:GLY:C	2.11	0.48
1:A:307:GLU:CA	1:C:409:MET:HE1	2.34	0.48
1:A:383:VAL:HG13	1:A:385:ILE:CG2	2.43	0.48
1:A:333:ILE:HG12	1:A:372:ALA:CB	2.44	0.48
1:C:322:PHE:CB	1:C:338:ILE:HG22	2.37	0.48
1:C:351:ARG:NH2	1:C:354:ASP:CB	2.76	0.48
1:A:363:ASP:OD1	1:A:365:ARG:HG3	2.12	0.48
1:C:379:ALA:HB3	1:C:383:VAL:CG1	2.42	0.48
1:C:360:ASN:OD1	1:C:379:ALA:HB1	2.14	0.48
1:A:339:LEU:CD1	1:A:342:GLY:HA3	2.43	0.48
1:C:332:GLY:C	1:C:333:ILE:HD12	2.39	0.47
1:C:358:SER:HA	1:C:362:VAL:O	2.14	0.47
1:A:314:HIS:NE2	1:A:382:THR:HG21	2.29	0.47
1:A:333:ILE:O	1:A:355:GLN:HG3	2.13	0.47
1:C:405:ARG:NE	1:C:406:GLU:CG	2.76	0.47
1:A:311:ILE:HD11	1:A:349:GLU:CB	2.44	0.47
1:C:322:PHE:HA	1:C:338:ILE:HA	1.96	0.47
1:C:333:ILE:O	1:C:355:GLN:HA	2.14	0.47
1:A:342:GLY:O	1:A:344:ALA:N	2.40	0.47
1:C:360:ASN:HD21	1:C:383:VAL:HA	1.79	0.47
1:A:306:ARG:CZ	1:A:391:PRO:HD2	2.45	0.46
1:C:335:ILE:HD11	1:C:351:ARG:O	2.14	0.46
1:C:354:ASP:N	1:C:354:ASP:OD1	2.46	0.46
1:C:401:ILE:HA	1:C:404:LEU:CD2	2.45	0.46
1:A:381:GLN:OE1	1:A:381:GLN:N	2.48	0.46
1:A:365:ARG:HH12	1:C:407:GLN:HB2	1.79	0.46
1:C:351:ARG:HG2	1:C:389:TYR:CE1	2.50	0.46
1:C:333:ILE:HG12	1:C:372:ALA:CB	2.45	0.46
1:A:333:ILE:HG12	1:A:372:ALA:HB2	1.98	0.46
1:A:339:LEU:HD13	1:A:342:GLY:HA3	1.97	0.46
1:A:308:PRO:O	1:C:420:TRP:CD1	2.70	0.45
1:A:325:VAL:HG12	1:A:423:GLN:HB2	1.97	0.45
1:A:418:PRO:HB2	1:A:420:TRP:CE2	2.52	0.45
1:C:351:ARG:CZ	1:C:389:TYR:HD1	2.29	0.45
1:C:351:ARG:HD3	1:C:351:ARG:N	2.30	0.45
1:C:351:ARG:HH11	1:C:389:TYR:HA	1.80	0.45
1:A:335:ILE:HD12	1:A:354:ASP:HB2	1.98	0.45
1:C:335:ILE:HG12	1:C:354:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLU:CA	1:C:409:MET:CE	2.94	0.45
1:C:335:ILE:HD13	1:C:351:ARG:O	2.17	0.45
1:A:324:ILE:HD11	1:A:333:ILE:CG2	2.46	0.45
1:A:357:LEU:HD11	1:A:388:GLN:HB3	1.99	0.45
1:C:368:SER:OG	1:C:369:HIS:N	2.49	0.45
1:A:307:GLU:HA	1:C:409:MET:HE1	1.97	0.44
1:A:335:ILE:HD11	1:A:350:LEU:HD13	1.99	0.44
1:C:420:TRP:CD1	1:C:420:TRP:H	2.36	0.44
1:A:370:GLU:O	1:A:374:ILE:HG23	2.18	0.44
1:C:395:SER:O	1:C:398:GLU:HG2	2.18	0.44
1:A:325:VAL:HG12	1:A:423:GLN:CB	2.48	0.43
1:A:324:ILE:CG2	1:A:424:THR:HB	2.48	0.43
1:A:359:VAL:HG22	1:A:383:VAL:HG21	1.98	0.43
1:C:407:GLN:HE21	1:C:407:GLN:HB3	1.49	0.43
1:A:326:GLY:HA3	1:A:332:GLY:O	2.18	0.43
1:C:369:HIS:CD2	1:C:422:GLN:HB3	2.53	0.43
1:C:401:ILE:O	1:C:402:HIS:C	2.58	0.43
1:C:405:ARG:NH2	1:C:406:GLU:HB2	2.34	0.43
1:C:333:ILE:HD11	1:C:368:SER:O	2.19	0.43
1:A:305:PHE:CE1	1:A:392:GLU:OE1	2.73	0.42
1:A:381:GLN:CG	1:A:382:THR:N	2.72	0.42
1:C:374:ILE:HG13	1:C:375:ALA:H	1.84	0.42
1:C:404:LEU:HD12	1:C:408:LEU:HD11	2.01	0.42
1:C:399:ALA:O	1:C:403:ASP:N	2.39	0.42
1:A:324:ILE:HD11	1:A:333:ILE:HG23	2.01	0.42
1:A:308:PRO:HD3	1:A:388:GLN:NE2	2.35	0.42
1:C:404:LEU:O	1:C:408:LEU:HD12	2.18	0.42
1:C:422:GLN:HE21	1:C:422:GLN:HB2	1.67	0.42
1:A:305:PHE:CD1	1:A:305:PHE:N	2.88	0.42
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.80	0.42
1:A:371:GLN:O	1:A:372:ALA:C	2.62	0.42
1:A:312:VAL:HG22	1:A:384:THR:HG22	2.02	0.41
1:C:375:ALA:HB2	2:C:503:HOH:O	2.20	0.41
1:A:313:ILE:HD12	1:A:314:HIS:H	1.85	0.41
1:C:322:PHE:HB2	1:C:337:PHE:O	2.20	0.41
1:A:420:TRP:CD1	1:A:420:TRP:H	2.36	0.41
1:C:335:ILE:HG23	1:C:354:ASP:CG	2.46	0.41
1:C:323:ASN:ND2	1:C:425:ARG:HE	2.19	0.41
1:C:403:ASP:O	1:C:405:ARG:NH2	2.54	0.41
1:C:417:PHE:N	1:C:417:PHE:CD1	2.87	0.41
1:A:323:ASN:HD22	1:A:425:ARG:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:O	1:C:386:ILE:HA	2.21	0.40
1:C:379:ALA:CB	1:C:383:VAL:CG1	3.00	0.40
1:A:357:LEU:CD1	1:A:388:GLN:H	2.34	0.40
1:A:365:ARG:HH22	1:C:407:GLN:NE2	2.18	0.40
1:A:408:LEU:HD12	1:A:408:LEU:C	2.47	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	113/123 (92%)	106 (94%)	7 (6%)	0	100	100
1	C	115/123 (94%)	112 (97%)	3 (3%)	0	100	100
All	All	228/246 (93%)	218 (96%)	10 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	88/98 (90%)	83 (94%)	5 (6%)	18	49
1	C	87/98 (89%)	79 (91%)	8 (9%)	8	27
All	All	175/196 (89%)	162 (93%)	13 (7%)	13	38

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	PHE
1	A	306	ARG
1	A	318	THR
1	A	336	SER
1	A	417	PHE
1	C	314	HIS
1	C	315	ARG
1	C	317	SER
1	C	336	SER
1	C	347	SER
1	C	368	SER
1	C	421	VAL
1	C	424	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	407	GLN
1	C	323	ASN
1	C	355	GLN
1	C	360	ASN
1	C	402	HIS
1	C	407	GLN
1	C	422	GLN
1	C	423	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	117/123 (95%)	1.32	35 (29%) 1 1	48, 78, 113, 139	0
1	C	119/123 (96%)	1.13	23 (19%) 3 2	56, 77, 110, 124	0
All	All	236/246 (95%)	1.22	58 (24%) 2 1	48, 78, 111, 139	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	GLY	4.3
1	A	339	LEU	3.8
1	A	338	ILE	3.5
1	C	342	GLY	3.4
1	A	346	LEU	3.4
1	C	313	ILE	3.3
1	C	308	PRO	3.2
1	C	410	ASN	3.0
1	C	316	GLY	3.0
1	A	344	ALA	3.0
1	C	343	PRO	3.0
1	A	359	VAL	3.0
1	C	324	ILE	2.8
1	A	370	GLU	2.8
1	C	329	ASP	2.8
1	A	332	GLY	2.8
1	A	327	GLY	2.7
1	A	330	GLY	2.7
1	A	325	VAL	2.7
1	A	378	ASN	2.7
1	A	313	ILE	2.6
1	A	319	GLY	2.6
1	A	318	THR	2.6
1	A	362	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	337	PHE	2.6
1	A	317	SER	2.6
1	A	340	ALA	2.6
1	C	340	ALA	2.5
1	C	358	SER	2.5
1	C	317	SER	2.5
1	A	380	GLY	2.4
1	A	417	PHE	2.4
1	A	418	PRO	2.4
1	A	341	GLY	2.4
1	C	319	GLY	2.4
1	C	369	HIS	2.3
1	A	360	ASN	2.3
1	A	356	ILE	2.3
1	C	318	THR	2.3
1	A	374	ILE	2.3
1	C	356	ILE	2.3
1	A	321	GLY	2.3
1	C	305	PHE	2.3
1	C	379	ALA	2.3
1	A	328	GLU	2.2
1	A	363	ASP	2.2
1	A	401	ILE	2.2
1	A	316	GLY	2.2
1	A	348	GLY	2.2
1	C	345	ASP	2.2
1	C	424	THR	2.2
1	C	371	GLN	2.1
1	A	358	SER	2.1
1	A	419	PRO	2.1
1	C	330	GLY	2.1
1	A	399	ALA	2.1
1	A	324	ILE	2.0
1	A	368	SER	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 [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.