



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:24 PM UTC

PDB ID : 3FGA / pdb_00003fga
Title : Structural Basis of PP2A and Sgo interaction
Authors : Xu, Z.; Xu, W.
Deposited on : 2008-12-05
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

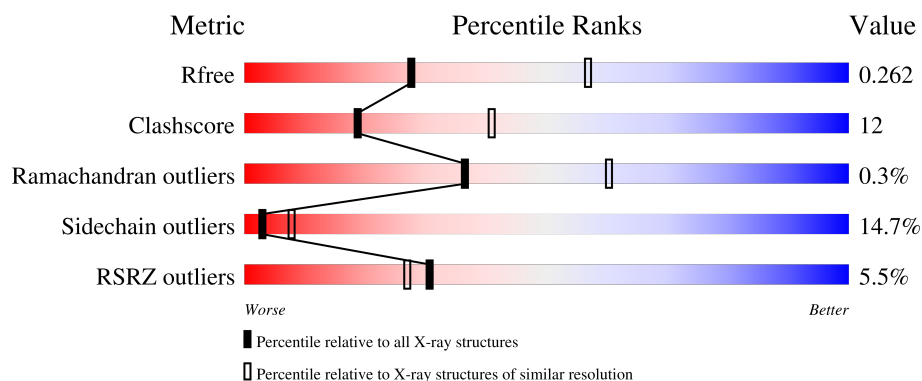
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	588	11% 71%24%5%
2	B	403	11% 67%26%7%
3	C	309	5% 62%29%6%
4	D	47	11% 74%26%
5	E	7	29% 29%29%14%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10810 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4532	2881	764	860	27			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3287	2149	540	582	16			

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	0
			2446	1549	421	461	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	ASN	ASP	engineered mutation	UNP P67775

- Molecule 4 is a protein called Shugoshin-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	47	Total	C	N	O	S	0	0	0
			380	239	64	74	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	50	PRO	-	insertion	UNP Q5FBB7

- Molecule 5 is a protein called MICROCYSTIN-LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	7	Total	C	N	O	0	0	0
			71	49	10	12			

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Mn	0	0
			2	2		

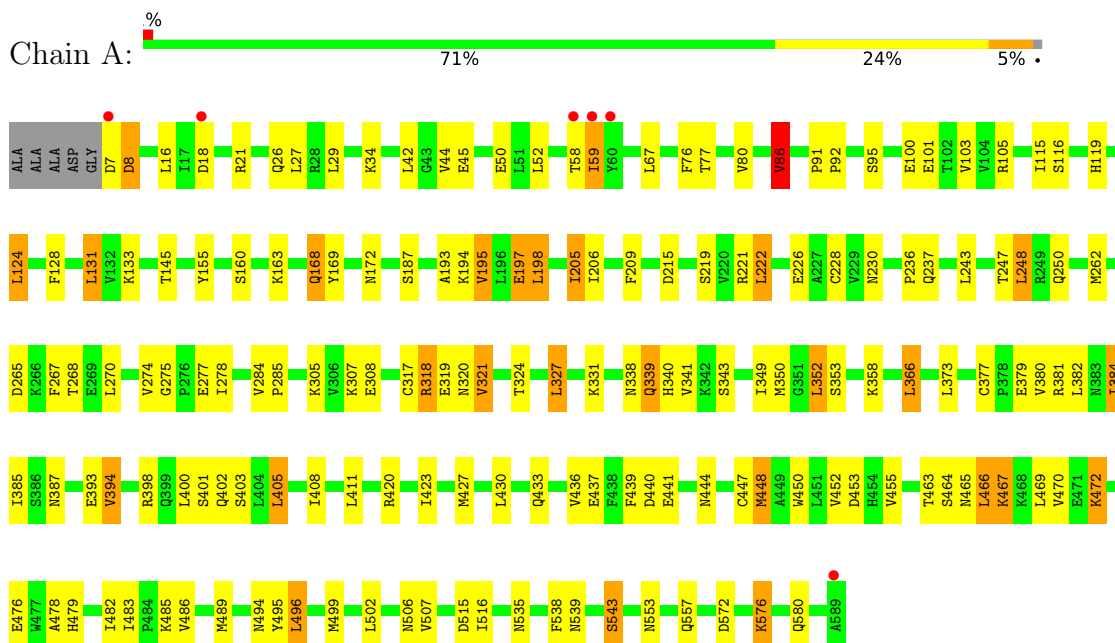
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total	O	0	0
			36	36		
7	B	11	Total	O	0	0
			11	11		
7	C	44	Total	O	0	0
			44	44		
7	D	1	Total	O	0	0
			1	1		

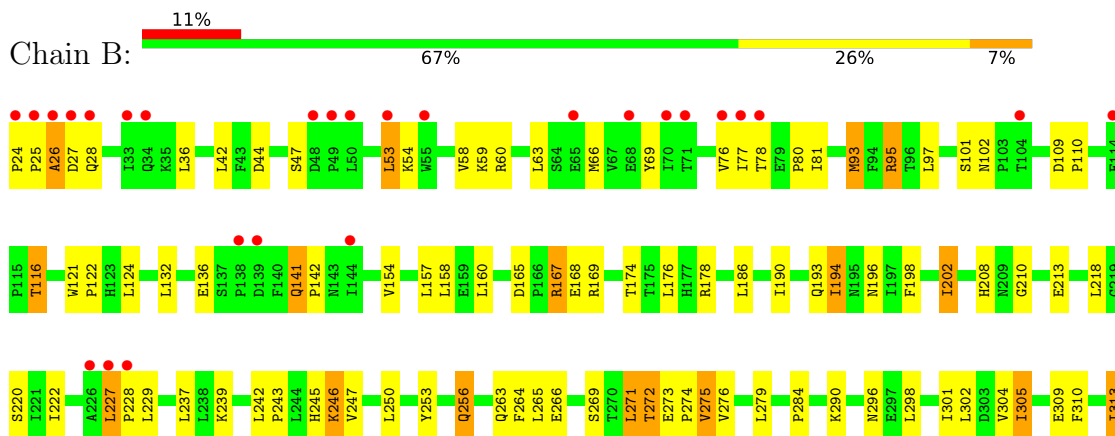
3 Residue-property plots

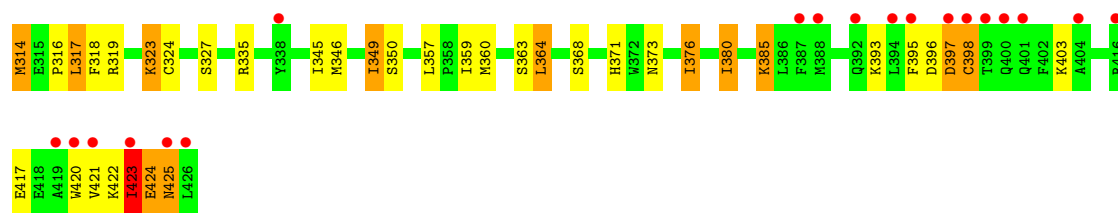
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

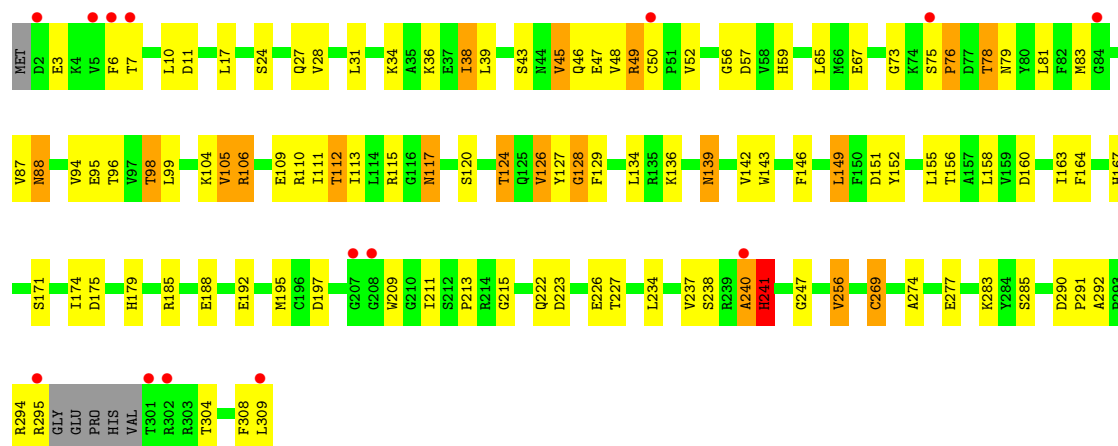


- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

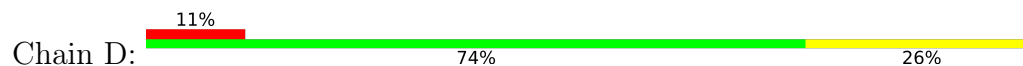




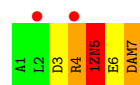
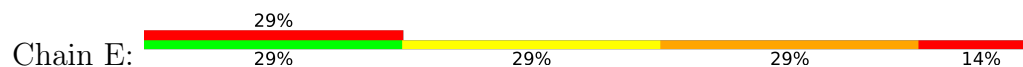
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



- Molecule 4: Shugoshin-like 1



- Molecule 5: MICROCYSTIN-LR



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.94Å 145.86Å 294.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.70 49.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (49.03-2.70) 92.7 (49.03-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.277 0.220 , 0.262	Depositor DCC
R_{free} test set	2898 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACB, FGA, 1ZN, DAL, DAM, MN

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	0.66	3/4606 (0.1%)	0.97	10/6255 (0.2%)
2	B	0.59	0/3378	0.97	10/4582 (0.2%)
3	C	0.64	0/2505	1.04	14/3396 (0.4%)
4	D	0.57	0/382	0.93	0/510
5	E	0.39	0/17	0.86	0/19
All	All	0.63	3/10888 (0.0%)	0.99	34/14762 (0.2%)

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
5	E	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	ASP	CA-C	-12.71	1.40	1.53
1	A	7	ASP	C-N	9.10	1.41	1.33
1	A	8	ASP	C-N	6.70	1.42	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	241	HIS	N-CA-C	10.42	125.73	112.92
2	B	425	ASN	N-CA-C	9.79	123.79	109.69
3	C	87	VAL	CA-C-N	-9.12	109.04	121.71
3	C	87	VAL	C-N-CA	-9.12	109.04	121.71
2	B	397	ASP	N-CA-C	-9.02	95.05	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	87	VAL	N-CA-C	8.11	121.66	113.47
3	C	128	GLY	N-CA-C	7.74	122.00	112.64
3	C	88	ASN	N-CA-C	7.19	124.51	110.56
2	B	424	GLU	N-CA-C	-7.03	97.38	108.63
3	C	241	HIS	N-CA-CB	-6.86	100.55	110.56
2	B	26	ALA	N-CA-C	6.82	125.32	110.80
1	A	8	ASP	CA-C-N	6.71	131.85	121.19
1	A	8	ASP	C-N-CA	6.71	131.85	121.19
3	C	269	CYS	N-CA-C	6.23	119.98	112.38
1	A	86	VAL	CB-CA-C	-6.07	103.18	112.05
2	B	425	ASN	N-CA-CB	-5.99	101.82	110.87
1	A	319	GLU	N-CA-C	5.95	117.44	111.07
3	C	50	CYS	N-CA-C	5.79	120.62	112.75
2	B	424	GLU	CA-C-O	-5.74	114.42	121.02
1	A	267	PHE	N-CA-C	5.73	117.61	111.36
3	C	240	ALA	CA-C-N	-5.72	113.50	122.65
3	C	240	ALA	C-N-CA	-5.72	113.50	122.65
1	A	275	GLY	CA-C-N	5.66	126.04	119.47
1	A	275	GLY	C-N-CA	5.66	126.04	119.47
2	B	424	GLU	CB-CA-C	5.52	119.72	110.88
1	A	198	LEU	N-CA-C	5.52	117.30	111.28
3	C	241	HIS	CB-CA-C	5.40	119.69	110.56
2	B	227	LEU	N-CA-C	5.36	121.66	109.81
1	A	8	ASP	CA-C-O	-5.10	114.48	121.98
2	B	26	ALA	N-CA-CB	-5.09	101.89	110.49
2	B	423	ILE	O-C-N	5.08	127.00	121.87
1	A	318	ARG	CB-CA-C	-5.04	100.40	110.42
3	C	50	CYS	CA-C-N	-5.03	114.25	120.79
3	C	50	CYS	C-N-CA	-5.03	114.25	120.79

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	4	ARG	Sidechain,Peptide
5	E	5	1ZN	Peptide,Mainchain

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	4532	0	4628	93	0
2	B	3287	0	3232	94	0
3	C	2446	0	2335	69	0
4	D	380	0	398	3	0
5	E	71	0	63	6	0
6	C	2	0	0	0	0
7	A	36	0	0	0	0
7	B	11	0	0	0	0
7	C	44	0	0	1	0
7	D	1	0	0	0	0
All	All	10810	0	10656	254	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 12.

All (254) 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)
3:C:269:CYS:SG	5:E:7:DAM:CB	2.25	1.24
3:C:94:VAL:O	3:C:98:THR:HG22	1.59	1.02
3:C:124:THR:CG2	3:C:143:TRP:HE1	1.73	1.01
2:B:208:HIS:HD2	2:B:210:GLY:H	1.09	0.99
3:C:269:CYS:SG	5:E:7:DAM:HB1	2.12	0.87
3:C:94:VAL:O	3:C:98:THR:CG2	2.24	0.85
3:C:124:THR:HG21	3:C:143:TRP:HE1	1.40	0.85
2:B:36:LEU:HD23	2:B:66:MET:HE1	1.57	0.85
1:A:353:SER:HB3	1:A:394:VAL:HG11	1.57	0.84
3:C:24:SER:H	3:C:27:GLN:HE21	1.24	0.83
1:A:274:VAL:CG1	1:A:278:ILE:HB	2.11	0.81
2:B:208:HIS:CD2	2:B:210:GLY:H	1.96	0.81
3:C:167:HIS:NE2	3:C:241:HIS:HB2	1.96	0.80
3:C:175:ASP:H	3:C:179:HIS:HD2	1.29	0.78
2:B:218:LEU:O	2:B:222:ILE:HG12	1.84	0.77
2:B:93:MET:HE1	2:B:124:LEU:HD22	1.67	0.77
3:C:167:HIS:CE1	3:C:241:HIS:HB2	2.18	0.76
2:B:269:SER:O	2:B:272:THR:HG23	1.86	0.75
4:D:89:CYS:O	4:D:93:THR:HG22	1.88	0.74
2:B:385:LYS:HG3	4:D:93:THR:HG21	1.71	0.73
1:A:499:MET:HE2	1:A:539:ASN:ND2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:O	2:B:63:LEU:HD23	1.90	0.71
3:C:139:ASN:C	3:C:139:ASN:HD22	1.99	0.70
1:A:274:VAL:HG13	1:A:278:ILE:HB	1.72	0.69
1:A:494:ASN:ND2	1:A:496:LEU:H	1.90	0.69
2:B:101:SER:HB2	2:B:116:THR:HG21	1.74	0.69
2:B:227:LEU:CB	2:B:228:PRO:CD	2.71	0.68
3:C:38:ILE:HD11	3:C:104:LYS:HE3	1.75	0.68
1:A:401:SER:HA	1:A:405:LEU:HB2	1.75	0.67
2:B:396:ASP:C	2:B:398:CYS:H	2.03	0.67
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.25	0.67
2:B:371:HIS:CE1	2:B:376:ILE:HD11	2.30	0.66
2:B:364:LEU:HD22	2:B:364:LEU:H	1.61	0.66
1:A:467:LYS:HB2	1:A:507:VAL:HG13	1.76	0.66
3:C:79:ASN:HD21	3:C:110:ARG:HD3	1.61	0.65
3:C:79:ASN:ND2	3:C:110:ARG:HD3	2.12	0.65
2:B:276:VAL:HG11	2:B:313:ILE:HG13	1.78	0.65
2:B:26:ALA:C	2:B:28:GLN:H	2.05	0.64
2:B:424:GLU:N	2:B:424:GLU:CD	2.56	0.64
3:C:24:SER:H	3:C:27:GLN:NE2	1.95	0.64
1:A:320:ASN:O	1:A:324:THR:HG22	1.97	0.64
1:A:486:VAL:HA	1:A:489:MET:HE3	1.78	0.64
1:A:427:MET:HG3	1:A:450:TRP:CH2	2.32	0.64
3:C:152:TYR:O	3:C:185:ARG:NH2	2.29	0.64
1:A:339:GLN:H	1:A:339:GLN:HE21	1.46	0.64
3:C:49:ARG:CD	3:C:49:ARG:H	2.12	0.63
1:A:494:ASN:HD22	1:A:495:TYR:N	1.96	0.63
3:C:73:GLY:HA3	3:C:78:THR:HG21	1.80	0.62
3:C:49:ARG:H	3:C:49:ARG:HD2	1.64	0.62
3:C:124:THR:HG21	3:C:143:TRP:NE1	2.12	0.62
2:B:26:ALA:C	2:B:28:GLN:N	2.55	0.61
3:C:126:VAL:HG22	3:C:127:TYR:CE2	2.36	0.61
1:A:427:MET:CE	1:A:439:PHE:HE2	2.14	0.61
1:A:494:ASN:HD22	1:A:494:ASN:C	2.09	0.61
3:C:10:LEU:HD11	3:C:105:VAL:HG22	1.82	0.60
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.82	0.60
1:A:427:MET:HE1	1:A:439:PHE:HE2	1.66	0.60
3:C:308:PHE:O	3:C:309:LEU:HB2	2.02	0.60
1:A:268:THR:HG21	1:A:308:GLU:HB3	1.84	0.60
3:C:215:GLY:HA3	5:E:5:1ZN:H14	1.83	0.60
3:C:213:PRO:HB2	5:E:4:ARG:HH11	1.67	0.59
3:C:98:THR:HB	3:C:146:PHE:HZ	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:PHE:HB2	3:C:234:LEU:HD13	1.84	0.59
1:A:91:PRO:HB2	1:A:92:PRO:HD3	1.85	0.59
1:A:381:ARG:O	1:A:385:ILE:HG12	2.03	0.59
2:B:165:ASP:OD2	2:B:167:ARG:HD3	2.03	0.59
2:B:213:GLU:OE2	2:B:213:GLU:N	2.28	0.59
2:B:265:LEU:HD22	2:B:272:THR:HG22	1.85	0.58
1:A:317:CYS:O	1:A:321:VAL:HG12	2.03	0.58
2:B:227:LEU:CB	2:B:228:PRO:HD3	2.33	0.58
3:C:11:ASP:OD1	3:C:106:ARG:HD2	2.04	0.58
2:B:424:GLU:CD	2:B:424:GLU:H	2.10	0.58
3:C:43:SER:H	3:C:46:GLN:HE21	1.52	0.58
2:B:304:VAL:HG12	2:B:304:VAL:O	2.03	0.57
2:B:222:ILE:HD12	2:B:264:PHE:CE1	2.39	0.57
2:B:318:PHE:HB2	2:B:359:ILE:HD11	1.85	0.57
1:A:339:GLN:H	1:A:339:GLN:NE2	2.02	0.57
2:B:93:MET:HA	2:B:93:MET:HE3	1.86	0.57
1:A:265:ASP:O	1:A:305:LYS:NZ	2.38	0.57
3:C:167:HIS:CD2	3:C:241:HIS:HB2	2.40	0.56
1:A:193:ALA:HB2	1:A:205:ILE:HD12	1.86	0.56
1:A:226:GLU:HG2	1:A:262:MET:HE2	1.86	0.56
1:A:572:ASP:OD2	3:C:110:ARG:NH1	2.38	0.56
1:A:576:LYS:HG2	1:A:580:GLN:HE21	1.70	0.56
3:C:45:VAL:HB	3:C:156:THR:OG1	2.06	0.56
3:C:167:HIS:O	3:C:241:HIS:HB3	2.06	0.56
1:A:506:ASN:ND2	1:A:543:SER:OG	2.39	0.56
2:B:373:ASN:HD22	2:B:376:ILE:H	1.52	0.56
1:A:349:ILE:O	1:A:352:LEU:HB2	2.06	0.56
2:B:78:THR:O	2:B:81:ILE:HG13	2.07	0.55
2:B:36:LEU:CD2	2:B:66:MET:HE1	2.32	0.55
2:B:397:ASP:O	2:B:397:ASP:OD2	2.25	0.54
2:B:423:ILE:O	2:B:425:ASN:HB3	2.06	0.54
3:C:269:CYS:SG	5:E:7:DAM:CA	2.89	0.54
2:B:318:PHE:CB	2:B:359:ILE:HD11	2.36	0.54
3:C:73:GLY:HA3	3:C:78:THR:CG2	2.38	0.54
1:A:427:MET:HG3	1:A:450:TRP:HH2	1.71	0.54
2:B:44:ASP:OD2	2:B:47:SER:HB3	2.06	0.54
1:A:168:GLN:HE22	1:A:172:ASN:HD21	1.53	0.54
2:B:284:PRO:HG2	2:B:290:LYS:HB3	1.90	0.53
3:C:124:THR:CG2	3:C:143:TRP:NE1	2.58	0.53
2:B:194:ILE:HD11	2:B:218:LEU:HD21	1.90	0.53
2:B:345:ILE:O	2:B:349:ILE:HG12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:TYR:CE1	2:B:76:VAL:HG11	2.43	0.53
1:A:516:ILE:H	1:A:516:ILE:HD12	1.73	0.53
3:C:117:ASN:HD22	3:C:167:HIS:CD2	2.26	0.53
2:B:121:TRP:N	2:B:122:PRO:HD2	2.23	0.52
1:A:119:HIS:HB2	1:A:124:LEU:HD13	1.91	0.52
3:C:117:ASN:HD22	3:C:117:ASN:H	1.57	0.52
1:A:539:ASN:O	1:A:543:SER:HB2	2.09	0.52
3:C:48:VAL:HG22	3:C:112:THR:HG21	1.92	0.52
1:A:408:ILE:HG23	1:A:423:ILE:HD12	1.91	0.52
2:B:393:LYS:C	2:B:395:PHE:H	2.18	0.52
2:B:24:PRO:HB2	2:B:25:PRO:CD	2.40	0.52
2:B:190:ILE:O	2:B:194:ILE:HG23	2.09	0.52
2:B:396:ASP:C	2:B:398:CYS:N	2.62	0.51
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.91	0.51
3:C:126:VAL:HG22	3:C:127:TYR:CD2	2.45	0.51
1:A:470:VAL:HG22	1:A:478:ALA:HB2	1.92	0.51
1:A:338:ASN:ND2	1:A:340:HIS:H	2.09	0.51
1:A:427:MET:HE1	1:A:439:PHE:CE2	2.45	0.51
1:A:128:PHE:O	1:A:131:LEU:HB3	2.11	0.50
1:A:133:LYS:HD3	1:A:169:TYR:CZ	2.46	0.50
1:A:448:MET:HE1	1:A:482:ILE:HG23	1.93	0.50
2:B:169:ARG:HD2	2:B:213:GLU:OE1	2.12	0.50
2:B:319:ARG:O	2:B:323:LYS:HG2	2.12	0.50
2:B:271:LEU:O	2:B:275:VAL:HG13	2.12	0.50
3:C:36:LYS:HG3	3:C:149:LEU:HD23	1.93	0.50
2:B:93:MET:CE	2:B:124:LEU:HD22	2.40	0.50
1:A:463:THR:O	1:A:466:LEU:HB2	2.12	0.49
2:B:360:MET:O	2:B:364:LEU:HD22	2.13	0.49
1:A:194:LYS:HE2	1:A:230:ASN:ND2	2.28	0.49
1:A:576:LYS:HG2	1:A:580:GLN:NE2	2.28	0.49
2:B:136:GLU:OE1	2:B:178:ARG:NH2	2.39	0.49
2:B:376:ILE:O	2:B:380:ILE:HG22	2.13	0.48
1:A:219:SER:HA	1:A:222:LEU:HD13	1.95	0.48
2:B:417:GLU:O	2:B:421:VAL:HG23	2.14	0.48
1:A:516:ILE:HD12	1:A:516:ILE:N	2.27	0.48
3:C:79:ASN:HD21	3:C:110:ARG:HH21	1.62	0.48
1:A:499:MET:HE3	1:A:535:ASN:C	2.39	0.48
1:A:101:GLU:OE2	2:B:246:LYS:NZ	2.46	0.48
1:A:385:ILE:HD11	1:A:411:LEU:HD13	1.95	0.47
2:B:193:GLN:NE2	2:B:196:ASN:HD22	2.12	0.47
3:C:83:MET:HE1	3:C:238:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:SER:CB	1:A:394:VAL:HG11	2.36	0.47
1:A:427:MET:HG3	1:A:450:TRP:CZ3	2.49	0.47
1:A:327:LEU:CD1	1:A:331:LYS:HE3	2.44	0.47
2:B:24:PRO:CB	2:B:25:PRO:CD	2.93	0.47
2:B:310:PHE:O	2:B:314:MET:HG2	2.14	0.47
1:A:59:ILE:HG23	1:A:59:ILE:O	2.14	0.47
1:A:366:LEU:HD21	1:A:403:SER:HB3	1.97	0.47
3:C:120:SER:HB2	3:C:188:GLU:OE2	2.15	0.47
1:A:350:MET:HE3	1:A:387:ASN:HB3	1.96	0.47
1:A:440:ASP:HA	1:A:444:ASN:HB2	1.97	0.47
2:B:26:ALA:O	2:B:28:GLN:N	2.47	0.47
3:C:88:ASN:HD22	3:C:129:PHE:H	1.62	0.47
1:A:197:GLU:CD	1:A:197:GLU:H	2.23	0.47
2:B:53:LEU:HD22	2:B:53:LEU:H	1.80	0.47
1:A:268:THR:HG21	1:A:308:GLU:CB	2.45	0.46
2:B:273:GLU:HB3	2:B:274:PRO:HD3	1.97	0.46
1:A:499:MET:CE	1:A:539:ASN:ND2	2.74	0.46
1:A:366:LEU:HD21	1:A:403:SER:CB	2.46	0.46
1:A:77:THR:HG23	1:A:86:VAL:HG13	1.97	0.46
1:A:350:MET:HE1	1:A:384:ILE:O	2.16	0.46
2:B:371:HIS:HE1	2:B:376:ILE:HD11	1.76	0.46
3:C:155:LEU:HD21	3:C:195:MET:HE3	1.98	0.46
1:A:350:MET:CE	1:A:384:ILE:O	2.64	0.46
2:B:305:ILE:HG12	2:B:310:PHE:HB2	1.97	0.46
1:A:494:ASN:HD21	1:A:496:LEU:HB2	1.80	0.46
1:A:553:ASN:O	1:A:557:GLN:HB2	2.16	0.45
2:B:313:ILE:O	2:B:316:PRO:HD2	2.15	0.45
2:B:368:SER:HA	2:B:380:ILE:HD11	1.98	0.45
2:B:242:LEU:O	2:B:245:HIS:HB2	2.15	0.45
2:B:121:TRP:CD1	2:B:167:ARG:NH1	2.84	0.45
2:B:296:ASN:HD22	2:B:335:ARG:HE	1.65	0.45
3:C:6:PHE:CE1	3:C:34:LYS:HD2	2.51	0.45
1:A:34:LYS:HD2	2:B:420:TRP:HZ2	1.81	0.45
2:B:313:ILE:O	2:B:317:LEU:HB2	2.15	0.45
3:C:56:GLY:HA2	3:C:240:ALA:HB1	1.99	0.45
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.51	0.45
3:C:17:LEU:HD13	3:C:99:LEU:HA	1.99	0.45
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.98	0.45
1:A:155:TYR:CE2	1:A:163:LYS:HE3	2.52	0.45
2:B:253:TYR:O	2:B:256:GLN:HG2	2.16	0.45
3:C:222:GLN:HG2	3:C:226:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ARG:NH1	1:A:453:ASP:OD1	2.50	0.44
1:A:472:LYS:HB3	1:A:472:LYS:HE3	1.65	0.44
1:A:194:LYS:HE2	1:A:230:ASN:HD22	1.82	0.44
1:A:447:CYS:HA	1:A:450:TRP:CE3	2.52	0.44
3:C:139:ASN:C	3:C:139:ASN:ND2	2.70	0.44
2:B:24:PRO:HB2	2:B:25:PRO:HD2	1.98	0.44
2:B:296:ASN:ND2	2:B:335:ARG:HH21	2.16	0.44
1:A:133:LYS:HD3	1:A:169:TYR:CE1	2.52	0.44
2:B:198:PHE:O	2:B:202:ILE:HG23	2.17	0.44
3:C:209:TRP:CB	4:D:65:VAL:HG21	2.48	0.44
1:A:284:VAL:HB	1:A:285:PRO:HD3	2.00	0.43
1:A:494:ASN:ND2	1:A:494:ASN:C	2.75	0.43
2:B:346:MET:HA	2:B:349:ILE:HG13	1.99	0.43
3:C:213:PRO:CB	5:E:4:ARG:HH11	2.31	0.43
1:A:248:LEU:HD11	1:A:270:LEU:HD22	2.00	0.43
2:B:202:ILE:CD1	2:B:246:LYS:HD3	2.49	0.43
3:C:95:GLU:OE2	3:C:136:LYS:HE2	2.19	0.43
1:A:206:ILE:HG21	1:A:243:LEU:HB3	2.00	0.43
1:A:494:ASN:ND2	1:A:496:LEU:HB2	2.34	0.43
2:B:109:ASP:HA	2:B:110:PRO:HD2	1.89	0.43
2:B:250:LEU:HD23	2:B:290:LYS:HG2	1.99	0.43
3:C:128:GLY:HA3	7:C:335:HOH:O	2.18	0.43
2:B:36:LEU:HD23	2:B:66:MET:CE	2.40	0.43
2:B:242:LEU:HB2	2:B:243:PRO:HD3	2.00	0.42
3:C:237:VAL:O	3:C:256:VAL:HA	2.18	0.42
1:A:433:GLN:HE21	1:A:433:GLN:HB2	1.63	0.42
1:A:499:MET:HE3	1:A:535:ASN:O	2.19	0.42
1:A:193:ALA:C	1:A:195:VAL:H	2.26	0.42
2:B:78:THR:C	2:B:80:PRO:HD2	2.44	0.42
3:C:171:SER:HB2	3:C:197:ASP:HB2	2.02	0.42
2:B:314:MET:O	2:B:318:PHE:HD1	2.03	0.42
2:B:95:ARG:NH2	2:B:168:GLU:OE1	2.48	0.42
3:C:104:LYS:HA	3:C:111:ILE:CG2	2.50	0.42
1:A:209:PHE:CE1	1:A:228:CYS:HB2	2.55	0.42
3:C:6:PHE:CZ	3:C:34:LYS:HD2	2.55	0.42
2:B:298:LEU:HA	2:B:301:ILE:HD12	2.01	0.42
2:B:54:LYS:O	2:B:58:VAL:HG23	2.19	0.41
1:A:237:GLN:HE21	1:A:237:GLN:HB3	1.74	0.41
2:B:349:ILE:HG12	2:B:349:ILE:H	1.73	0.41
2:B:121:TRP:N	2:B:122:PRO:CD	2.82	0.41
1:A:8:ASP:OD2	1:A:8:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:O	1:A:119:HIS:HD2	2.03	0.41
1:A:479:HIS:HA	1:A:483:ILE:HG13	2.01	0.41
2:B:36:LEU:CD2	2:B:66:MET:CE	2.98	0.41
2:B:279:LEU:HD12	2:B:298:LEU:HD13	2.01	0.41
2:B:141:GLN:HE21	2:B:141:GLN:HB2	1.64	0.41
3:C:65:LEU:HD22	3:C:96:THR:HG23	2.03	0.41
1:A:116:SER:HA	1:A:119:HIS:CD2	2.55	0.41
2:B:271:LEU:O	2:B:275:VAL:CG1	2.68	0.41
3:C:48:VAL:CG2	3:C:112:THR:HG21	2.51	0.41
3:C:88:ASN:ND2	3:C:129:PHE:H	2.19	0.41
1:A:100:GLU:O	1:A:105:ARG:NH1	2.53	0.41
1:A:215:ASP:O	1:A:221:ARG:HD3	2.21	0.41
1:A:506:ASN:HD21	1:A:543:SER:HA	1.85	0.41
2:B:132:LEU:HA	2:B:132:LEU:HD23	1.89	0.41
2:B:243:PRO:C	2:B:245:HIS:N	2.78	0.41
3:C:75:SER:N	3:C:76:PRO:CD	2.84	0.41
3:C:115:ARG:NH1	3:C:151:ASP:HA	2.35	0.41
1:A:236:PRO:O	1:A:237:GLN:C	2.63	0.41
1:A:499:MET:CE	1:A:539:ASN:HD22	2.34	0.41
1:A:168:GLN:HE22	1:A:172:ASN:ND2	2.18	0.40
2:B:178:ARG:HD3	2:B:178:ARG:HA	1.81	0.40
2:B:271:LEU:O	2:B:274:PRO:HD2	2.22	0.40
2:B:368:SER:CA	2:B:380:ILE:HD11	2.50	0.40
2:B:165:ASP:OD1	2:B:167:ARG:NH2	2.54	0.40
3:C:57:ASP:HB3	3:C:59:HIS:CD2	2.57	0.40
3:C:247:GLY:O	3:C:274:ALA:HB3	2.22	0.40
1:A:377:CYS:SG	1:A:380:VAL:HG23	2.61	0.40
2:B:324:CYS:O	2:B:327:SER:HB3	2.21	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	581/588 (99%)	557 (96%)	24 (4%)	0	100	100
2	B	401/403 (100%)	379 (94%)	19 (5%)	3 (1%)	18	41
3	C	299/309 (97%)	282 (94%)	16 (5%)	1 (0%)	36	60
4	D	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
5	E	1/7 (14%)	1 (100%)	0	0	100	100
All	All	1327/1354 (98%)	1262 (95%)	61 (5%)	4 (0%)	36	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	27	ASP
3	C	76	PRO
2	B	77	ILE
2	B	142	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	506/511 (99%)	432 (85%)	74 (15%)	3	8
2	B	353/375 (94%)	303 (86%)	50 (14%)	3	8
3	C	265/274 (97%)	226 (85%)	39 (15%)	3	8
4	D	44/45 (98%)	35 (80%)	9 (20%)	1	3
5	E	2/2 (100%)	2 (100%)	0	100	100
All	All	1170/1207 (97%)	998 (85%)	172 (15%)	3	8

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	18	ASP
1	A	21	ARG
1	A	26	GLN

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	29	LEU
1	A	42	LEU
1	A	44	VAL
1	A	45	GLU
1	A	50	GLU
1	A	52	LEU
1	A	58	THR
1	A	59	ILE
1	A	67	LEU
1	A	76	PHE
1	A	80	VAL
1	A	86	VAL
1	A	95	SER
1	A	103	VAL
1	A	124	LEU
1	A	131	LEU
1	A	145	THR
1	A	160	SER
1	A	168	GLN
1	A	187	SER
1	A	195	VAL
1	A	197	GLU
1	A	198	LEU
1	A	205	ILE
1	A	222	LEU
1	A	247	THR
1	A	248	LEU
1	A	250	GLN
1	A	277	GLU
1	A	307	LYS
1	A	318	ARG
1	A	321	VAL
1	A	327	LEU
1	A	339	GLN
1	A	341	VAL
1	A	343	SER
1	A	352	LEU
1	A	358	LYS
1	A	366	LEU
1	A	373	LEU
1	A	379	GLU

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Mol	Chain	Res	Type
1	A	382	LEU
1	A	384	ILE
1	A	393	GLU
1	A	394	VAL
1	A	398	ARG
1	A	400	LEU
1	A	402	GLN
1	A	405	LEU
1	A	430	LEU
1	A	436	VAL
1	A	437	GLU
1	A	441	GLU
1	A	448	MET
1	A	452	VAL
1	A	455	VAL
1	A	464	SER
1	A	465	ASN
1	A	466	LEU
1	A	467	LYS
1	A	469	LEU
1	A	472	LYS
1	A	476	GLU
1	A	485	LYS
1	A	496	LEU
1	A	502	LEU
1	A	515	ASP
1	A	543	SER
1	A	576	LYS
2	B	42	LEU
2	B	53	LEU
2	B	60	ARG
2	B	93	MET
2	B	95	ARG
2	B	97	LEU
2	B	102	ASN
2	B	116	THR
2	B	141	GLN
2	B	154	VAL
2	B	157	LEU
2	B	158	LEU
2	B	160	LEU
2	B	167	ARG

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Mol	Chain	Res	Type
2	B	174	THR
2	B	176	LEU
2	B	186	LEU
2	B	194	ILE
2	B	202	ILE
2	B	220	SER
2	B	229	LEU
2	B	237	LEU
2	B	239	LYS
2	B	246	LYS
2	B	247	VAL
2	B	256	GLN
2	B	263	GLN
2	B	266	GLU
2	B	271	LEU
2	B	272	THR
2	B	275	VAL
2	B	302	LEU
2	B	305	ILE
2	B	309	GLU
2	B	313	ILE
2	B	314	MET
2	B	317	LEU
2	B	323	LYS
2	B	349	ILE
2	B	350	SER
2	B	357	LEU
2	B	363	SER
2	B	364	LEU
2	B	376	ILE
2	B	380	ILE
2	B	385	LYS
2	B	398	CYS
2	B	403	LYS
2	B	422	LYS
2	B	423	ILE
3	C	3	GLU
3	C	7	THR
3	C	31	LEU
3	C	38	ILE
3	C	39	LEU
3	C	45	VAL

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Mol	Chain	Res	Type
3	C	47	GLU
3	C	49	ARG
3	C	52	VAL
3	C	78	THR
3	C	81	LEU
3	C	98	THR
3	C	105	VAL
3	C	106	ARG
3	C	109	GLU
3	C	112	THR
3	C	113	ILE
3	C	117	ASN
3	C	124	THR
3	C	126	VAL
3	C	134	LEU
3	C	139	ASN
3	C	149	LEU
3	C	158	LEU
3	C	160	ASP
3	C	163	ILE
3	C	174	ILE
3	C	192	GLU
3	C	211	ILE
3	C	223	ASP
3	C	227	THR
3	C	241	HIS
3	C	256	VAL
3	C	277	GLU
3	C	283	LYS
3	C	285	SER
3	C	294	ARG
3	C	295	ARG
3	C	304	THR
4	D	52	THR
4	D	53	LEU
4	D	54	LEU
4	D	58	GLN
4	D	63	MET
4	D	68	LEU
4	D	74	LYS
4	D	79	GLN
4	D	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	30	ASN
1	A	119	HIS
1	A	172	ASN
1	A	211	ASN
1	A	217	GLN
1	A	230	ASN
1	A	237	GLN
1	A	250	GLN
1	A	312	ASN
1	A	325	GLN
1	A	338	ASN
1	A	339	GLN
1	A	360	ASN
1	A	387	ASN
1	A	392	ASN
1	A	399	GLN
1	A	433	GLN
1	A	454	HIS
1	A	465	ASN
1	A	494	ASN
1	A	506	ASN
1	A	520	HIS
1	A	580	GLN
2	B	87	HIS
2	B	141	GLN
2	B	193	GLN
2	B	208	HIS
2	B	223	ASN
2	B	233	HIS
2	B	254	HIS
2	B	296	ASN
2	B	329	HIS
2	B	331	GLN
2	B	341	ASN
2	B	373	ASN
2	B	382	ASN
2	B	392	GLN
3	C	27	GLN
3	C	46	GLN
3	C	63	HIS

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Mol	Chain	Res	Type
3	C	79	ASN
3	C	88	ASN
3	C	139	ASN
3	C	162	GLN
3	C	179	HIS
3	C	272	GLN
4	D	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FGA	E	6	5	6,8,9	2.49	2 (33%)	6,9,11	0.43	0
5	1ZN	E	5	5	21,23,24	1.20	2 (9%)	25,29,31	0.83	0
5	DAM	E	7	5	4,5,6	1.82	1 (25%)	3,5,7	4.10	2 (66%)
5	ACB	E	3	5	7,8,9	2.92	3 (42%)	8,10,12	1.75	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FGA	E	6	5	-	3/8/8/9	-
5	1ZN	E	5	5	-	1/23/25/27	0/1/1/1
5	DAM	E	7	5	-	0/0/4/6	-
5	ACB	E	3	5	-	4/10/10/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	6	FGA	O-C	5.10	1.37	1.22
5	E	3	ACB	O-C	4.81	1.36	1.22
5	E	3	ACB	CA-N	4.58	1.60	1.47
5	E	3	ACB	OXT-C	-3.26	1.20	1.30
5	E	7	DAM	C-CA	3.08	1.50	1.45
5	E	6	FGA	OXT-C	-2.57	1.22	1.30
5	E	5	1ZN	C5-C4	2.36	1.43	1.38
5	E	5	1ZN	C3-C2	2.23	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	7	DAM	O-C-CA	-5.33	118.40	125.33
5	E	7	DAM	CM-N-CA	-4.46	117.22	123.98
5	E	3	ACB	O-C-CA	-3.08	111.30	121.72
5	E	3	ACB	OXT-C-CA	3.01	124.54	114.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3	ACB	C4-CB-CG-OD1
5	E	6	FGA	OXT-C-CA-N
5	E	3	ACB	OXT-C-CA-N
5	E	3	ACB	CA-CB-CG-OD1
5	E	5	1ZN	C10-C2-C3-C4
5	E	6	FGA	CA-CB-CG-CD
5	E	3	ACB	O-C-CA-N
5	E	6	FGA	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	5	1ZN	1	0
5	E	7	DAM	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	583/588 (99%)	-0.08	6 (1%) 79 78	29, 42, 62, 77	0
2	B	403/403 (100%)	0.59	46 (11%) 10 8	31, 55, 90, 103	0
3	C	303/309 (98%)	-0.08	14 (4%) 37 34	24, 38, 55, 84	0
4	D	47/47 (100%)	0.58	5 (10%) 11 9	37, 49, 74, 83	0
5	E	2/7 (28%)	4.56	2 (100%) 0 0	91, 91, 91, 103	0
All	All	1338/1354 (98%)	0.15	73 (5%) 30 27	24, 44, 81, 103	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	227	LEU	5.7
2	B	395	PHE	5.0
5	E	4	ARG	4.9
2	B	426	LEU	4.8
2	B	394	LEU	4.7
2	B	24	PRO	4.7
1	A	60	TYR	4.6
5	E	2	LEU	4.3
2	B	48	ASP	4.1
2	B	228	PRO	4.1
3	C	309	LEU	4.1
3	C	2	ASP	3.9
2	B	27	ASP	3.8
4	D	50	PRO	3.8
2	B	419	ALA	3.8
2	B	420	TRP	3.7
3	C	240	ALA	3.7
2	B	226	ALA	3.6
2	B	50	LEU	3.6
2	B	25	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	423	ILE	3.4
2	B	33	ILE	3.3
3	C	50	CYS	3.3
2	B	77	ILE	3.2
2	B	421	VAL	3.1
1	A	58	THR	3.1
2	B	28	GLN	3.0
2	B	34	GLN	3.0
2	B	144	ILE	3.0
1	A	589	ALA	3.0
2	B	404	ALA	3.0
4	D	52	THR	3.0
4	D	53	LEU	2.9
2	B	388	MET	2.8
2	B	70	ILE	2.8
3	C	301	THR	2.8
1	A	59	ILE	2.8
3	C	207	GLY	2.8
2	B	26	ALA	2.8
2	B	392	GLN	2.8
2	B	400	GLN	2.7
2	B	76	VAL	2.7
3	C	84	GLY	2.7
2	B	53	LEU	2.7
3	C	208	GLY	2.7
2	B	78	THR	2.5
2	B	401	GLN	2.6
3	C	75	SER	2.5
4	D	51	SER	2.5
1	A	7	ASP	2.5
2	B	416	ARG	2.5
2	B	114	GLU	2.4
2	B	49	PRO	2.4
3	C	6	PHE	2.4
3	C	302	ARG	2.4
2	B	399	THR	2.4
2	B	387	PHE	2.3
2	B	104	THR	2.3
2	B	425	ASN	2.3
2	B	138	PRO	2.3
3	C	295	ARG	2.3
4	D	54	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	397	ASP	2.2
2	B	71	THR	2.2
2	B	65	GLU	2.2
3	C	7	THR	2.2
1	A	18	ASP	2.2
2	B	338	TYR	2.1
3	C	5	VAL	2.1
2	B	68	GLU	2.1
2	B	55	TRP	2.0
2	B	398	CYS	2.0
2	B	139	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FGA	E	6	9/10	0.81	0.25	81,90,97,100	0
5	DAM	E	7	6/7	0.81	0.29	76,80,81,82	0
5	DAL	E	1	5/6	0.86	0.24	77,77,80,80	0
5	1ZN	E	5	23/24	0.89	0.25	64,70,89,93	0
5	ACB	E	3	9/10	0.90	0.22	93,97,99,101	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MN	C	311	1/1	0.96	0.05	48,48,48,48	0
6	MN	C	312	1/1	0.99	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.