



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 08:01 PM UTC

PDB ID : 3CHG / pdb_00003chg
Title : The compatible solute-binding protein OpuAC from *Bacillus subtilis* in complex with DMSA
Authors : Smits, S.H.J.; Hoing, M.; Lecher, J.; Jebbar, M.; Schmitt, L.; Bremer, E.
Deposited on : 2008-03-09
Resolution : 2.80 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

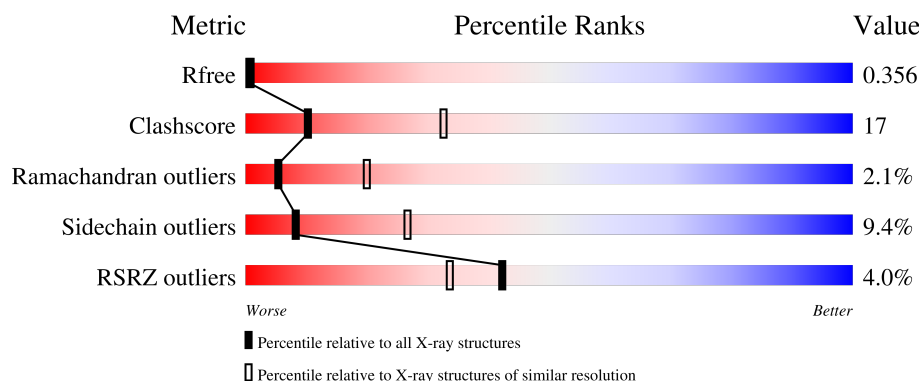
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	268	0% 65% 30% • •
1	B	268	4% 69% 24% • • •
1	C	268	4% 60% 30% 7% •
1	D	268	6% 53% 34% 7% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	313	A	4	-	X	-	-

2 Entry composition [i](#)

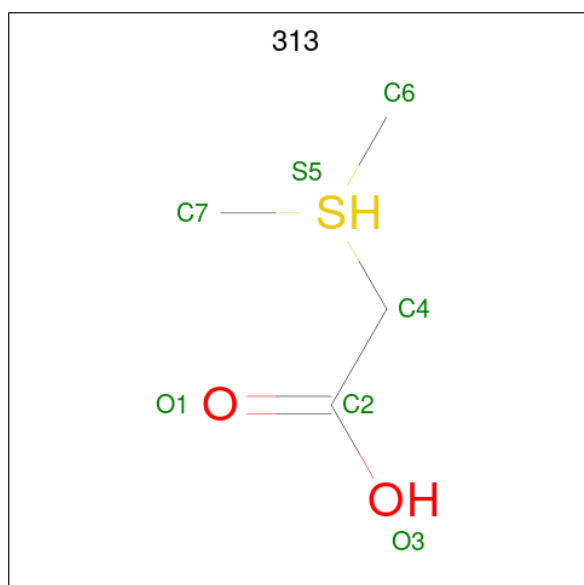
There are 2 unique types of molecules in this entry. The entry contains 8104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycine betaine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	257	Total	C	N	O	S	0	1	0
			2019	1290	331	387	11			
1	A	258	Total	C	N	O	S	0	0	0
			2019	1289	332	388	10			
1	B	258	Total	C	N	O	S	0	0	0
			2019	1289	332	388	10			
1	C	258	Total	C	N	O	S	0	0	0
			2019	1289	332	388	10			

- Molecule 2 is (dimethyl-lambda 4 -sulfanyl)acetic acid (CCD ID: 313) (formula: C₄H₁₀O₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	S	0	0
			7	4	2	1		
2	A	1	Total	C	O	S	0	0
			7	4	2	1		

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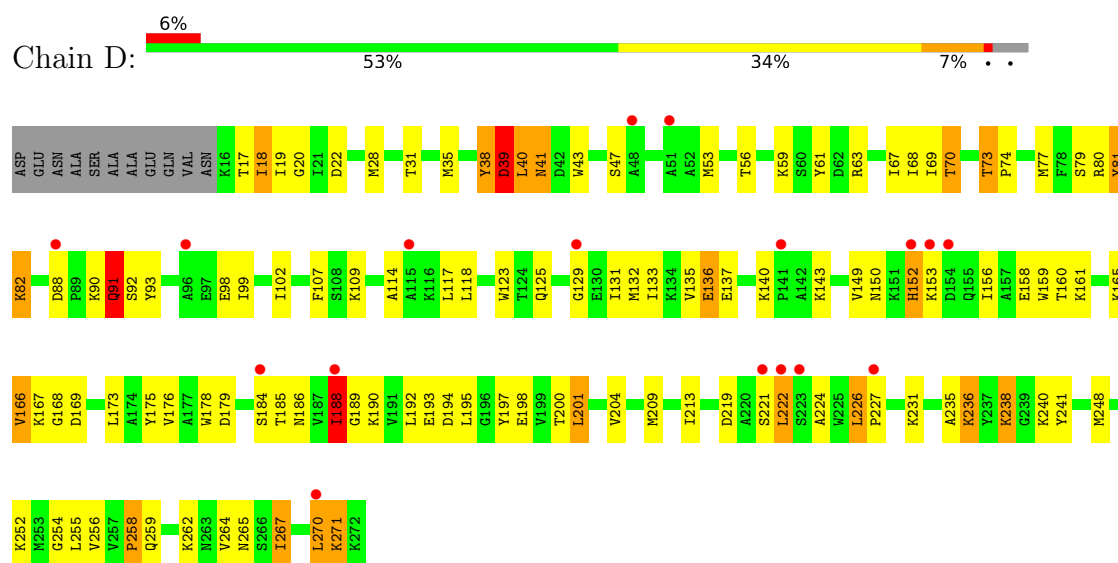
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	S	0	0
			7	4	2	1		
2	C	1	Total	C	O	S	0	0
			7	4	2	1		

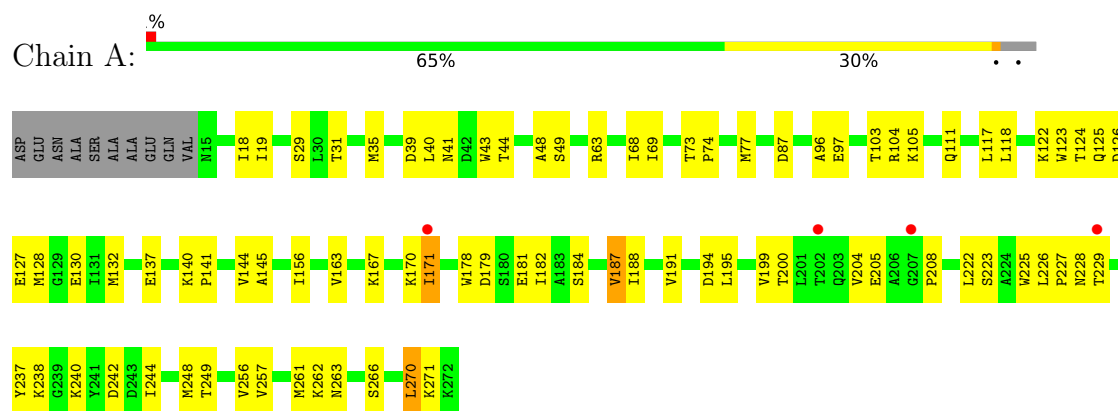
3 Residue-property plots

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.

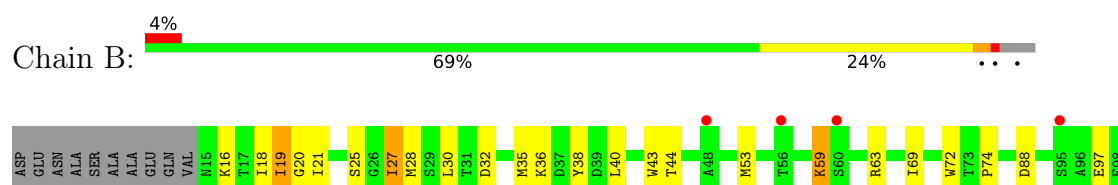
• Molecule 1: Glycine betaine-binding protein

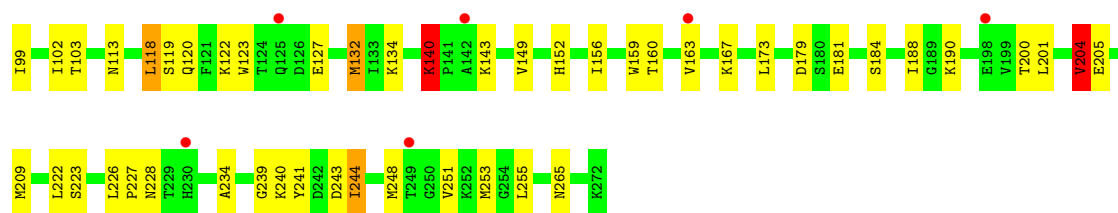


• Molecule 1: Glycine betaine-binding protein

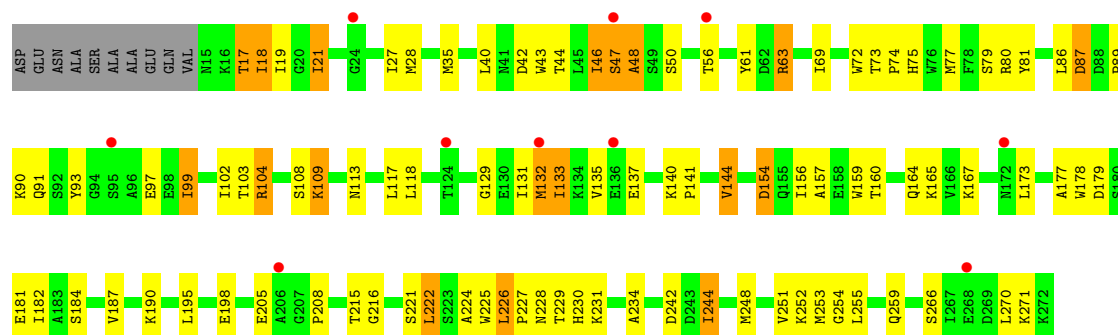


• Molecule 1: Glycine betaine-binding protein





● Molecule 1: Glycine betaine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.51Å 150.61Å 58.96Å 90.00° 104.54° 90.00°	Depositor
Resolution (Å)	19.56 – 2.80 19.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.56-2.80) 92.8 (19.56-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.285 , 0.359 0.289 , 0.356	Depositor DCC
R_{free} test set	1119 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8104	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8216e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
313

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	0.51	0/2062	0.87	0/2786
1	B	0.50	0/2062	0.84	2/2786 (0.1%)
1	C	0.48	0/2062	0.83	2/2786 (0.1%)
1	D	0.72	5/2062 (0.2%)	0.85	8/2785 (0.3%)
All	All	0.56	5/8248 (0.1%)	0.85	12/11143 (0.1%)

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	3
1	D	0	10
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	LYS	CA-C	-6.46	1.44	1.52
1	D	219	ASP	C-N	-5.78	1.26	1.33
1	D	91	GLN	CA-C	-5.70	1.45	1.52
1	D	235	ALA	CA-CB	-5.63	1.43	1.53
1	D	136	GLU	C-O	-5.07	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	241	TYR	O-C-N	-6.45	115.68	123.10
1	D	226	LEU	C-N-CD	-6.08	107.23	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	ASP	CA-C-N	6.04	125.52	119.24
1	D	22	ASP	C-N-CA	6.04	125.52	119.24
1	D	241	TYR	CA-C-N	5.98	131.43	123.00
1	D	241	TYR	C-N-CA	5.98	131.43	123.00
1	C	140	LYS	CA-C-N	5.69	126.95	119.84
1	C	140	LYS	C-N-CA	5.69	126.95	119.84
1	D	136	GLU	N-CA-C	5.51	119.72	112.89
1	D	235	ALA	N-CA-C	5.29	118.99	112.54
1	B	140	LYS	CA-C-N	5.09	124.75	119.56
1	B	140	LYS	C-N-CA	5.09	124.75	119.56

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	132	MET	Peptide
1	C	46	ILE	Peptide
1	C	47	SER	Peptide
1	D	168	GLY	Peptide
1	D	188	ILE	Peptide
1	D	200	THR	Peptide
1	D	201	LEU	Peptide
1	D	258	PRO	Peptide
1	D	270	LEU	Peptide
1	D	271	LYS	Peptide
1	D	38	TYR	Peptide
1	D	39	ASP	Peptide
1	D	40	LEU	Peptide

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	2019	0	2034	38	1
1	B	2019	0	2034	42	0
1	C	2019	0	2034	70	0
1	D	2019	0	2036	131	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	7	0	9	0	0
2	B	7	0	9	1	0
2	C	7	0	9	3	0
2	D	7	0	9	2	0
All	All	8104	0	8174	279	2

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 17.

All (279) 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:D:114:ALA:O	1:D:118:LEU:HD13	1.19	1.33
1:C:132:MET:O	1:C:133:ILE:HG13	1.36	1.21
1:D:270:LEU:HD13	1:D:270:LEU:O	1.44	1.17
1:D:74:PRO:HB3	1:D:125:GLN:HG3	1.17	1.15
1:D:114:ALA:O	1:D:118:LEU:CD1	1.94	1.15
1:D:150:ASN:O	1:D:153:LYS:HD2	1.56	1.05
1:D:188:ILE:HD13	1:D:222:LEU:HD21	1.38	1.03
1:D:166:VAL:HG11	1:D:197:TYR:CE1	1.96	1.00
1:D:74:PRO:HB3	1:D:125:GLN:CG	1.93	0.99
1:C:132:MET:O	1:C:133:ILE:CG1	2.14	0.95
1:D:18:ILE:HD13	1:D:68:ILE:HB	1.49	0.94
1:D:166:VAL:HG11	1:D:197:TYR:CD1	2.05	0.91
1:D:40:LEU:HD23	1:D:271:LYS:HD2	1.52	0.90
1:D:150:ASN:O	1:D:153:LYS:CD	2.19	0.89
1:D:166:VAL:CG1	1:D:197:TYR:CE1	2.57	0.86
1:D:184:SER:O	1:D:188:ILE:CG2	2.23	0.86
1:C:21:ILE:O	1:C:47:SER:O	1.92	0.86
1:D:184:SER:O	1:D:188:ILE:HG22	1.75	0.86
1:D:20:GLY:HA2	1:D:70:THR:OG1	1.75	0.85
1:D:74:PRO:CB	1:D:125:GLN:HG3	2.05	0.84
1:D:188:ILE:HD13	1:D:222:LEU:CD2	2.08	0.83
1:D:166:VAL:CG1	1:D:197:TYR:CD1	2.61	0.82
1:A:184:SER:O	1:A:187:VAL:HG12	1.81	0.81
1:C:28:MET:HE1	1:C:46:ILE:O	1.79	0.81
1:B:99:ILE:CG2	1:B:248:MET:HB2	2.11	0.81
1:A:237:TYR:HD1	1:A:240:LYS:HD2	1.45	0.81
1:D:18:ILE:HD13	1:D:68:ILE:CB	2.12	0.79
1:D:59:LYS:HA	1:D:63:ARG:HH21	1.48	0.79
1:D:118:LEU:CD1	1:D:118:LEU:H	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:THR:CG2	1:C:252:LYS:HB2	2.16	0.76
1:C:18:ILE:HD11	1:C:255:LEU:CD2	2.16	0.75
1:C:46:ILE:HG22	1:C:47:SER:H	1.50	0.75
1:C:102:ILE:HD11	1:C:221:SER:HB3	1.69	0.74
1:D:213:ILE:HD11	1:D:221:SER:HB2	1.68	0.74
1:C:18:ILE:HD11	1:C:255:LEU:HD22	1.68	0.74
1:D:61:TYR:CE1	1:D:81:TYR:HB3	2.22	0.74
1:D:38:TYR:O	1:D:39:ASP:HB2	1.85	0.74
1:C:73:THR:HG22	1:C:252:LYS:HB2	1.70	0.73
1:D:270:LEU:O	1:D:270:LEU:CD1	2.30	0.73
1:D:129:GLY:O	1:D:133:ILE:HG13	1.88	0.73
1:D:188:ILE:CD1	1:D:222:LEU:HD21	2.16	0.73
1:D:222:LEU:N	1:D:222:LEU:HD12	2.02	0.73
1:D:226:LEU:HB3	1:D:227:PRO:HA	1.70	0.73
1:B:99:ILE:HG22	1:B:248:MET:HB2	1.70	0.72
1:D:150:ASN:C	1:D:153:LYS:HD2	2.14	0.72
1:D:114:ALA:C	1:D:118:LEU:HD13	2.10	0.72
1:D:118:LEU:N	1:D:118:LEU:HD12	2.04	0.71
1:D:40:LEU:O	1:D:43:TRP:HB2	1.90	0.71
1:C:17:THR:HG22	1:C:18:ILE:H	1.56	0.71
1:C:108:SER:O	1:C:109:LYS:HB2	1.90	0.70
1:D:166:VAL:CG2	1:D:167:LYS:N	2.54	0.70
1:D:158:GLU:HG2	1:D:161:LYS:NZ	2.07	0.70
1:C:113:ASN:HD21	1:C:164:GLN:H	1.39	0.70
1:D:43:TRP:CZ2	1:D:270:LEU:HD13	2.27	0.69
1:D:149:VAL:O	1:D:153:LYS:HG2	1.92	0.69
1:D:18:ILE:HD12	1:D:255:LEU:HD22	1.74	0.69
1:D:193:GLU:O	1:D:195:LEU:N	2.26	0.68
1:A:87:ASP:HB2	1:A:266:SER:HA	1.73	0.68
1:D:173:LEU:HB2	1:D:201:LEU:HD12	1.76	0.68
1:D:43:TRP:CZ2	1:D:270:LEU:CD1	2.77	0.68
1:A:237:TYR:CD1	1:A:240:LYS:HD2	2.28	0.68
1:D:59:LYS:HA	1:D:63:ARG:NH2	2.07	0.68
1:D:173:LEU:HB2	1:D:201:LEU:CD1	2.23	0.68
1:D:188:ILE:O	1:D:192:LEU:HB2	1.94	0.67
1:D:73:THR:HG22	1:D:252:LYS:H	1.60	0.67
1:A:48:ALA:O	1:A:49:SER:HB3	1.94	0.67
1:D:186:ASN:ND2	1:D:201:LEU:HD21	2.10	0.66
1:C:141:PRO:HA	1:C:144:VAL:HG12	1.77	0.66
1:D:118:LEU:CD1	1:D:118:LEU:N	2.58	0.66
1:D:140:LYS:HB2	1:D:143:LYS:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ASP:CG	1:D:91:GLN:HA	2.21	0.66
1:D:18:ILE:HD13	1:D:68:ILE:CG2	2.27	0.65
1:D:99:ILE:HA	1:D:224:ALA:O	1.95	0.65
1:D:61:TYR:CD2	1:D:81:TYR:HD1	2.15	0.65
1:D:193:GLU:C	1:D:195:LEU:H	2.04	0.64
1:D:222:LEU:N	1:D:222:LEU:CD1	2.61	0.63
1:C:117:LEU:HD11	1:C:160:THR:HG22	1.80	0.63
1:D:20:GLY:HA3	1:D:28:MET:HE1	1.81	0.63
1:D:18:ILE:CD1	1:D:68:ILE:CG2	2.77	0.63
1:B:59:LYS:O	1:B:59:LYS:HG2	1.97	0.63
1:D:136:GLU:HG3	1:D:136:GLU:O	1.99	0.62
1:B:181:GLU:HG2	1:B:223:SER:HA	1.82	0.62
1:D:166:VAL:HG22	1:D:167:LYS:N	2.15	0.61
1:D:88:ASP:OD2	1:D:91:GLN:HA	2.00	0.61
1:A:68:ILE:HG13	1:A:257:VAL:HG12	1.81	0.61
1:D:209:MET:SD	1:D:221:SER:OG	2.58	0.60
1:D:61:TYR:CZ	1:D:81:TYR:HB3	2.36	0.60
1:D:18:ILE:CD1	1:D:68:ILE:HG21	2.31	0.60
1:A:171:ILE:HG23	1:A:171:ILE:O	1.99	0.60
1:C:132:MET:O	1:C:133:ILE:CB	2.49	0.59
1:B:205:GLU:O	1:B:209:MET:HB2	2.03	0.59
1:C:99:ILE:CG2	1:C:248:MET:HB3	2.32	0.59
1:C:102:ILE:CD1	1:C:221:SER:HB3	2.33	0.59
1:D:117:LEU:HG	1:D:160:THR:HG22	1.85	0.59
1:C:21:ILE:HG22	1:C:50:SER:HA	1.85	0.59
1:D:132[B]:MET:HE3	1:D:179:ASP:HA	1.84	0.58
1:B:102:ILE:HG22	1:B:243:ASP:HA	1.84	0.58
1:D:166:VAL:HG11	1:D:197:TYR:CZ	2.36	0.58
1:C:35:MET:HA	1:C:40:LEU:HB2	1.85	0.58
1:D:131:ILE:O	1:D:135:VAL:HG23	2.05	0.57
1:C:117:LEU:HD13	1:C:195:LEU:HD11	1.85	0.57
1:B:35:MET:HA	1:B:40:LEU:HD12	1.86	0.57
1:D:40:LEU:CD2	1:D:271:LYS:HD2	2.31	0.57
1:D:90:LYS:O	1:D:91:GLN:C	2.47	0.57
1:C:99:ILE:HD11	1:C:222:LEU:O	2.05	0.57
1:D:150:ASN:C	1:D:153:LYS:HG3	2.30	0.57
1:D:150:ASN:HA	1:D:153:LYS:HD2	1.87	0.57
1:A:69:ILE:HG12	1:A:256:VAL:O	2.03	0.57
1:D:166:VAL:HG12	1:D:197:TYR:CE1	2.38	0.56
1:C:97:GLU:HB3	1:C:251:VAL:HG23	1.86	0.56
1:C:154:ASP:OD2	1:C:154:ASP:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:GLU:C	1:D:195:LEU:N	2.62	0.56
1:D:43:TRP:CH2	1:D:270:LEU:HD11	2.40	0.56
1:D:118:LEU:H	1:D:118:LEU:HD12	1.63	0.56
1:D:150:ASN:CA	1:D:153:LYS:HD2	2.36	0.56
1:C:225:TRP:HB3	1:C:229:THR:CG2	2.36	0.55
1:D:158:GLU:HG2	1:D:161:LYS:HZ2	1.72	0.55
1:D:213:ILE:CD1	1:D:221:SER:HB2	2.36	0.55
1:C:87:ASP:O	1:C:89:PRO:HD3	2.07	0.55
1:B:149:VAL:HG23	1:B:156:ILE:HG12	1.89	0.55
1:A:35:MET:HA	1:A:40:LEU:HB2	1.87	0.54
1:A:141:PRO:HA	1:A:144:VAL:HG12	1.87	0.54
1:D:40:LEU:HD11	1:D:267:ILE:HG22	1.90	0.54
1:D:73:THR:HG23	1:D:125:GLN:OE1	2.07	0.54
1:D:43:TRP:CZ2	1:D:270:LEU:HD11	2.42	0.54
1:B:156:ILE:HA	1:B:159:TRP:HB2	1.89	0.54
1:D:188:ILE:O	1:D:192:LEU:HD12	2.07	0.54
1:A:97:GLU:OE2	1:A:229:THR:HG22	2.08	0.54
1:B:226:LEU:HD21	1:B:234:ALA:HB2	1.90	0.54
1:C:18:ILE:HD11	1:C:255:LEU:HD21	1.90	0.53
1:A:43:TRP:HE1	1:A:271:LYS:HD3	1.74	0.53
1:A:156:ILE:H	1:A:156:ILE:HD12	1.73	0.53
1:D:188:ILE:HG21	1:D:222:LEU:CD2	2.39	0.53
1:D:166:VAL:HG23	1:D:167:LYS:H	1.73	0.53
1:A:226:LEU:HB3	1:A:227:PRO:HA	1.90	0.53
1:C:132:MET:C	1:C:133:ILE:HG13	2.24	0.52
1:B:103:THR:HG23	1:B:244:ILE:HD12	1.91	0.52
1:A:43:TRP:HZ2	1:A:270:LEU:O	1.92	0.52
1:A:68:ILE:HG13	1:A:257:VAL:CG1	2.40	0.51
1:D:238:LYS:C	1:D:240:LYS:H	2.17	0.51
1:D:118:LEU:HD13	1:D:118:LEU:H	1.74	0.51
1:A:178:TRP:O	1:A:182:ILE:HG13	2.10	0.51
1:D:149:VAL:HG23	1:D:156:ILE:HG12	1.93	0.51
1:D:166:VAL:CG2	1:D:167:LYS:H	2.23	0.51
1:D:150:ASN:C	1:D:153:LYS:CG	2.84	0.51
1:D:188:ILE:HG21	1:D:222:LEU:HD23	1.92	0.51
1:C:43:TRP:CZ2	1:C:270:LEU:HB3	2.46	0.51
1:A:181:GLU:HG2	1:A:223:SER:HA	1.93	0.50
1:C:103:THR:OG1	1:C:242:ASP:HB2	2.11	0.50
1:B:38:TYR:OH	1:B:88:ASP:OD2	2.29	0.50
1:C:69:ILE:O	1:C:255:LEU:HA	2.11	0.50
1:C:226:LEU:HD11	1:C:234:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:HA3	1:B:28:MET:HE1	1.94	0.50
1:A:117:LEU:HD12	1:A:163:VAL:HG11	1.94	0.50
1:B:32:ASP:O	1:B:36:LYS:HD2	2.11	0.49
1:C:19:ILE:HD13	1:C:56:THR:HG21	1.94	0.49
1:C:47:SER:O	1:C:48:ALA:O	2.30	0.49
1:A:74:PRO:HB2	1:A:132:MET:HE1	1.94	0.49
1:B:113:ASN:ND2	1:B:163:VAL:HG13	2.28	0.49
1:B:27:ILE:HG22	2:B:2:313:O3	2.12	0.49
1:B:113:ASN:HD21	1:B:163:VAL:HG13	1.77	0.49
1:B:127:GLU:HG2	1:B:152:HIS:HE1	1.77	0.49
1:C:74:PRO:HB2	1:C:132:MET:HE1	1.95	0.49
1:C:184:SER:O	1:C:187:VAL:HG12	2.12	0.49
1:C:72:TRP:NE1	2:C:3:313:H7	2.28	0.49
1:C:93:TYR:CE1	1:C:254:GLY:HA2	2.48	0.49
1:B:241:TYR:HE1	1:B:243:ASP:HB2	1.79	0.48
1:B:16:LYS:HB3	1:B:43:TRP:CD2	2.49	0.48
1:D:150:ASN:HA	1:D:153:LYS:CD	2.44	0.48
1:D:61:TYR:CD2	1:D:81:TYR:CD1	3.00	0.48
1:D:176:VAL:HG23	1:D:209:MET:HG3	1.95	0.48
1:D:59:LYS:HG2	1:D:63:ARG:HH21	1.79	0.48
1:C:72:TRP:HA	1:C:253:MET:HA	1.96	0.47
1:C:117:LEU:CD1	1:C:195:LEU:HD11	2.43	0.47
1:D:82:LYS:O	1:D:259:GLN:HB2	2.15	0.47
1:C:87:ASP:C	1:C:89:PRO:HD3	2.39	0.47
1:A:125:GLN:HG2	1:A:248:MET:SD	2.54	0.47
1:A:127:GLU:O	1:A:130:GLU:HB2	2.14	0.47
1:C:72:TRP:CE2	2:C:3:313:H7	2.49	0.47
1:C:79:SER:O	1:C:80:ARG:HG2	2.15	0.47
1:B:226:LEU:HB3	1:B:227:PRO:HA	1.97	0.47
1:D:150:ASN:C	1:D:153:LYS:CD	2.83	0.47
1:D:175:TYR:HB3	1:D:185:THR:HG21	1.96	0.47
1:D:226:LEU:HB3	1:D:227:PRO:CA	2.42	0.47
1:B:127:GLU:HG2	1:B:152:HIS:CE1	2.49	0.47
1:D:38:TYR:OH	1:D:88:ASP:OD1	2.25	0.47
1:D:158:GLU:C	1:D:160:THR:N	2.73	0.46
1:D:133:ILE:O	1:D:137:GLU:HG2	2.15	0.46
1:C:75:HIS:ND1	1:C:77:MET:HB2	2.30	0.46
1:A:31:THR:O	1:A:35:MET:HG3	2.16	0.46
1:A:103:THR:OG1	1:A:242:ASP:HB2	2.14	0.46
1:D:262:LYS:O	1:D:265:ASN:ND2	2.45	0.46
1:A:39:ASP:HA	1:A:41:ASN:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ASP:O	1:D:271:LYS:CE	2.64	0.46
1:D:43:TRP:CZ2	1:D:270:LEU:O	2.69	0.46
1:C:226:LEU:HB3	1:C:227:PRO:HA	1.98	0.46
1:D:186:ASN:ND2	1:D:201:LEU:CD2	2.78	0.46
1:B:25:SER:OG	1:B:28:MET:HB2	2.15	0.46
1:D:123:TRP:CZ2	1:D:184:SER:HB3	2.50	0.46
1:B:74:PRO:HD3	1:B:251:VAL:HG12	1.97	0.46
1:C:27:ILE:HD12	1:C:253:MET:HB2	1.97	0.46
1:D:90:LYS:O	1:D:92:SER:N	2.50	0.45
1:A:261:MET:C	1:A:263:ASN:H	2.23	0.45
1:B:30:LEU:HD12	1:B:253:MET:HE1	1.98	0.45
1:D:158:GLU:HG2	1:D:161:LYS:HZ1	1.78	0.45
1:D:80:ARG:HB3	1:D:81:TYR:CE2	2.52	0.45
1:D:123:TRP:HZ2	1:D:184:SER:HB3	1.81	0.45
1:D:192:LEU:O	1:D:193:GLU:C	2.60	0.45
1:D:123:TRP:O	1:D:248:MET:HG2	2.17	0.45
1:B:97:GLU:OE1	1:B:228:ASN:HB3	2.17	0.45
1:A:178:TRP:O	1:A:182:ILE:N	2.50	0.45
1:D:28:MET:HE2	1:D:47:SER:HA	1.98	0.45
1:B:132:MET:HE3	1:B:179:ASP:HA	1.99	0.45
1:C:87:ASP:HB2	1:C:266:SER:HA	1.99	0.45
1:D:93:TYR:CE1	1:D:254:GLY:HA2	2.52	0.44
1:C:61:TYR:CE1	1:C:81:TYR:HB3	2.52	0.44
1:C:156:ILE:HA	1:C:159:TRP:HB2	1.98	0.44
1:D:238:LYS:O	1:D:240:LYS:N	2.46	0.44
1:D:69:ILE:HG13	1:D:256:VAL:HB	2.00	0.44
1:D:166:VAL:HG21	1:D:169:ASP:HB2	1.99	0.44
1:A:205:GLU:HB2	1:A:208:PRO:HG2	2.00	0.44
1:D:77:MET:C	1:D:79:SER:H	2.25	0.43
1:A:122:LYS:O	1:A:123:TRP:HB3	2.18	0.43
1:C:108:SER:O	1:C:109:LYS:CB	2.62	0.43
1:C:225:TRP:HB3	1:C:229:THR:HG21	2.01	0.43
1:D:59:LYS:CA	1:D:63:ARG:HH21	2.26	0.43
1:D:178:TRP:CD2	2:D:1:313:H4A	2.53	0.43
1:C:205:GLU:HB2	1:C:208:PRO:HG2	2.00	0.43
1:B:19:ILE:HG23	1:B:69:ILE:HG22	1.99	0.43
1:B:21:ILE:HG21	1:B:72:TRP:HH2	1.84	0.43
1:C:129:GLY:O	1:C:133:ILE:HD12	2.19	0.43
1:A:96:ALA:HB2	1:C:48:ALA:N	2.34	0.43
1:B:134:LYS:HE3	1:C:63:ARG:HG2	2.01	0.43
1:C:102:ILE:HG12	1:C:224:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:O	1:C:135:VAL:HG23	2.19	0.42
1:C:225:TRP:HB3	1:C:229:THR:HG23	2.01	0.42
1:D:158:GLU:C	1:D:160:THR:H	2.27	0.42
1:A:145:ALA:HB1	1:A:187:VAL:HA	2.01	0.42
1:D:107:PHE:C	1:D:109:LYS:H	2.27	0.42
1:A:225:TRP:HB3	1:A:229:THR:CG2	2.49	0.42
1:C:46:ILE:HG22	1:C:47:SER:N	2.22	0.42
1:C:90:LYS:O	1:C:91:GLN:HB2	2.20	0.42
1:C:229:THR:HB	1:C:253:MET:HE1	2.01	0.42
1:A:191:VAL:O	1:A:195:LEU:HG	2.19	0.42
1:C:179:ASP:HA	1:C:182:ILE:HD12	2.02	0.42
1:B:59:LYS:HA	1:B:63:ARG:NH2	2.35	0.42
1:C:230:HIS:O	1:C:231:LYS:C	2.62	0.42
1:A:126:ASP:OD1	1:A:127:GLU:N	2.52	0.42
1:A:170:LYS:O	1:A:171:ILE:HB	2.18	0.42
1:D:19:ILE:HG22	1:D:53:MET:HG2	2.02	0.42
1:D:39:ASP:O	1:D:271:LYS:HE3	2.19	0.42
1:A:74:PRO:HG2	1:A:128:MET:SD	2.60	0.42
1:D:158:GLU:O	1:D:161:LYS:HG2	2.20	0.41
1:A:105:LYS:HD2	1:A:105:LYS:HA	1.88	0.41
1:C:72:TRP:CD1	2:C:3:313:H7	2.54	0.41
1:C:104:ARG:HH11	1:C:104:ARG:HB2	1.84	0.41
1:B:140:LYS:HB2	1:B:143:LYS:HG3	2.01	0.41
1:C:86:LEU:O	1:C:87:ASP:C	2.63	0.41
1:B:204:VAL:HB	1:B:205:GLU:H	1.59	0.41
1:D:67:ILE:HG23	1:D:258:PRO:HD3	2.02	0.41
1:B:122:LYS:O	1:B:123:TRP:HB3	2.20	0.41
1:D:59:LYS:O	1:D:63:ARG:NE	2.53	0.41
1:C:154:ASP:O	1:C:157:ALA:HB3	2.21	0.41
1:D:186:ASN:HD21	1:D:201:LEU:CD2	2.33	0.41
1:D:178:TRP:CE2	2:D:1:313:H4A	2.56	0.41
1:B:19:ILE:HD11	1:B:53:MET:HA	2.03	0.41
1:B:123:TRP:HZ2	1:B:184:SER:HB3	1.86	0.41
1:D:132[B]:MET:HE3	1:D:179:ASP:CA	2.49	0.41
1:B:173:LEU:HB2	1:B:201:LEU:HD23	2.02	0.41
1:A:111:GLN:HE22	1:A:171:ILE:HB	1.86	0.40
1:B:118:LEU:O	1:B:120:GLN:N	2.54	0.40
1:B:239:GLY:C	1:B:240:LYS:HG3	2.46	0.40
1:C:178:TRP:HB2	1:C:181:GLU:HB2	2.02	0.40
1:D:31:THR:O	1:D:35:MET:HG3	2.21	0.40
1:B:27:ILE:O	1:B:27:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ILE:HD13	1:B:188:ILE:HA	2.00	0.40
1:C:226:LEU:CB	1:C:227:PRO:HA	2.50	0.40
1:B:167:LYS:HA	1:B:167:LYS:HD3	1.78	0.40
1:C:244:ILE:H	1:C:244:ILE:HD13	1.85	0.40

All (2) 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:D:41:ASN:ND2	1:D:165:LYS:N[1_655]	2.05	0.15
1:D:236:LYS:NZ	1:A:104:ARG:NH2[2_656]	2.10	0.10

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	256/268 (96%)	226 (88%)	27 (10%)	3 (1%)	10	34
1	B	256/268 (96%)	235 (92%)	19 (7%)	2 (1%)	16	44
1	C	256/268 (96%)	219 (86%)	29 (11%)	8 (3%)	3	12
1	D	256/268 (96%)	216 (84%)	32 (12%)	8 (3%)	3	12
All	All	1024/1072 (96%)	896 (88%)	107 (10%)	21 (2%)	5	20

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	39	ASP
1	A	171	ILE
1	C	109	LYS
1	C	133	ILE
1	D	91	GLN

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Mol	Chain	Res	Type
1	D	189	GLY
1	D	194	ASP
1	D	238	LYS
1	C	18	ILE
1	A	262	LYS
1	D	152	HIS
1	C	216	GLY
1	D	231	LYS
1	A	238	LYS
1	B	119	SER
1	C	177	ALA
1	C	215	THR
1	D	159	TRP
1	C	48	ALA
1	B	204	VAL
1	C	21	ILE

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	216/223 (97%)	192 (89%)	24 (11%)	6	20
1	B	216/223 (97%)	200 (93%)	16 (7%)	13	37
1	C	216/223 (97%)	194 (90%)	22 (10%)	7	23
1	D	216/223 (97%)	197 (91%)	19 (9%)	9	29
All	All	864/892 (97%)	783 (91%)	81 (9%)	8	27

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	17	THR
1	D	18	ILE
1	D	41	ASN
1	D	56	THR
1	D	70	THR

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Mol	Chain	Res	Type
1	D	73	THR
1	D	81	TYR
1	D	82	LYS
1	D	98	GLU
1	D	102	ILE
1	D	152	HIS
1	D	166	VAL
1	D	188	ILE
1	D	190	LYS
1	D	198	GLU
1	D	204	VAL
1	D	222	LEU
1	D	264	VAL
1	D	267	ILE
1	A	18	ILE
1	A	19	ILE
1	A	29	SER
1	A	44	THR
1	A	63	ARG
1	A	73	THR
1	A	77	MET
1	A	118	LEU
1	A	124	THR
1	A	137	GLU
1	A	140	LYS
1	A	167	LYS
1	A	179	ASP
1	A	187	VAL
1	A	188	ILE
1	A	194	ASP
1	A	199	VAL
1	A	200	THR
1	A	204	VAL
1	A	222	LEU
1	A	228	ASN
1	A	244	ILE
1	A	249	THR
1	A	270	LEU
1	B	18	ILE
1	B	19	ILE
1	B	27	ILE
1	B	44	THR

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Mol	Chain	Res	Type
1	B	59	LYS
1	B	118	LEU
1	B	132	MET
1	B	140	LYS
1	B	160	THR
1	B	190	LYS
1	B	200	THR
1	B	204	VAL
1	B	222	LEU
1	B	244	ILE
1	B	255	LEU
1	B	265	ASN
1	C	17	THR
1	C	42	ASP
1	C	44	THR
1	C	63	ARG
1	C	87	ASP
1	C	99	ILE
1	C	104	ARG
1	C	118	LEU
1	C	137	GLU
1	C	144	VAL
1	C	154	ASP
1	C	165	LYS
1	C	167	LYS
1	C	173	LEU
1	C	190	LYS
1	C	198	GLU
1	C	222	LEU
1	C	226	LEU
1	C	228	ASN
1	C	244	ILE
1	C	259	GLN
1	C	271	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	91	GLN
1	D	100	HIS
1	D	111	GLN
1	D	113	ASN

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Mol	Chain	Res	Type
1	D	120	GLN
1	D	152	HIS
1	D	186	ASN
1	D	259	GLN
1	A	41	ASN
1	A	111	GLN
1	A	113	ASN
1	A	120	GLN
1	A	228	ASN
1	A	259	GLN
1	B	111	GLN
1	B	113	ASN
1	B	228	ASN
1	B	259	GLN
1	C	113	ASN
1	C	186	ASN

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](#)

4 ligands 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
2	313	A	4	-	5,6,6	4.23	2 (40%)	6,7,7	4.33	3 (50%)
2	313	C	3	-	5,6,6	4.12	2 (40%)	6,7,7	3.74	3 (50%)
2	313	D	1	-	5,6,6	4.21	2 (40%)	6,7,7	3.86	3 (50%)
2	313	B	2	-	5,6,6	4.14	2 (40%)	6,7,7	4.62	3 (50%)

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
2	313	A	4	-	-	2/4/4/4	-
2	313	C	3	-	-	0/4/4/4	-
2	313	D	1	-	-	0/4/4/4	-
2	313	B	2	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4	313	C6-S5	-6.61	1.66	1.78
2	D	1	313	C7-S5	-6.54	1.66	1.78
2	D	1	313	C6-S5	-6.52	1.66	1.78
2	A	4	313	C7-S5	-6.47	1.66	1.78
2	B	2	313	C7-S5	-6.46	1.66	1.78
2	C	3	313	C7-S5	-6.44	1.66	1.78
2	B	2	313	C6-S5	-6.33	1.66	1.78
2	C	3	313	C6-S5	-6.31	1.66	1.78

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	313	C6-S5-C7	7.04	110.72	101.48
2	B	2	313	C7-S5-C4	6.74	112.08	101.32
2	B	2	313	C6-S5-C4	6.64	111.92	101.32
2	C	3	313	C6-S5-C7	6.63	110.17	101.48
2	D	1	313	C6-S5-C7	6.26	109.70	101.48
2	A	4	313	C7-S5-C4	6.17	111.16	101.32
2	B	2	313	C6-S5-C7	5.70	108.95	101.48
2	D	1	313	C7-S5-C4	5.34	109.83	101.32
2	C	3	313	C6-S5-C4	5.07	109.40	101.32
2	A	4	313	C6-S5-C4	4.40	108.33	101.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	313	C6-S5-C4	4.10	107.87	101.32
2	C	3	313	C7-S5-C4	2.91	105.96	101.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4	313	C2-C4-S5-C7
2	A	4	313	C2-C4-S5-C6
2	B	2	313	C2-C4-S5-C6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	313	3	0
2	D	1	313	2	0
2	B	2	313	1	0

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	258/268 (96%)	0.55	4 (1%) 70 61	10, 16, 21, 24	0
1	B	258/268 (96%)	0.61	10 (3%) 43 34	9, 16, 22, 23	0
1	C	258/268 (96%)	0.60	10 (3%) 43 34	9, 15, 21, 23	0
1	D	257/268 (95%)	0.71	17 (6%) 24 18	8, 16, 20, 22	1 (0%)
All	All	1031/1072 (96%)	0.62	41 (3%) 42 33	8, 16, 21, 24	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	SER	3.6
1	D	96	ALA	3.2
1	C	95	SER	3.1
1	D	153	LYS	3.1
1	A	207	GLY	2.9
1	B	125	GLN	2.9
1	D	270	LEU	2.7
1	D	115	ALA	2.7
1	B	230	HIS	2.7
1	D	227	PRO	2.7
1	B	48	ALA	2.6
1	D	141	PRO	2.6
1	C	132	MET	2.5
1	D	222	LEU	2.5
1	C	268	GLU	2.5
1	D	51	ALA	2.4
1	C	124	THR	2.4
1	D	88	ASP	2.3
1	A	202	THR	2.3
1	A	229	THR	2.3
1	B	249	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	24	GLY	2.3
1	C	206	ALA	2.3
1	B	95	SER	2.3
1	B	56	THR	2.2
1	C	56	THR	2.2
1	C	172	ASN	2.2
1	D	152	HIS	2.2
1	B	163	VAL	2.2
1	A	171	ILE	2.2
1	C	47	SER	2.2
1	D	184	SER	2.1
1	D	188	ILE	2.1
1	D	223	SER	2.1
1	B	198	GLU	2.1
1	D	48	ALA	2.1
1	D	154	ASP	2.0
1	D	221	SER	2.0
1	D	129	GLY	2.0
1	B	142	ALA	2.0
1	C	136	GLU	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](#)

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
2	313	B	2	7/7	0.92	0.11	18,18,19,19	0
2	313	D	1	7/7	0.93	0.13	28,28,28,28	0
2	313	C	3	7/7	0.95	0.10	16,16,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	313	A	4	7/7	0.96	0.10	27,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.