



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:06 AM UTC

PDB ID : 6UBR / pdb_00006ubr
Title : Crystal structure of D678A GoxA bound to glycine at pH 7.5
Authors : Yukl, E.T.; Avalos, D.
Deposited on : 2019-09-12
Resolution : 1.96 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

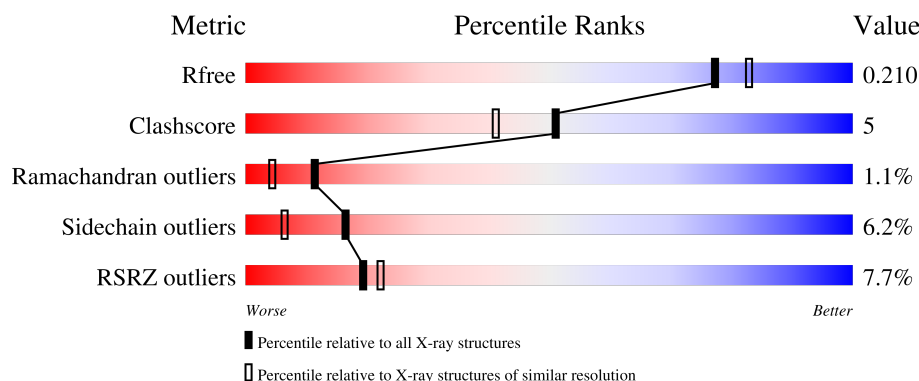
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	816	7% 82% 12% • •
1	B	816	7% 83% 11% • •
1	C	816	8% 82% 11% • 5%
1	D	816	8% 82% 11% • 5%

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
5	GLY	A	904	-	-	X	-
5	GLY	C	902	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 50448 atoms, of which 23513 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	782	Total	C	H	N	O	S	0	2	0
			12073	3921	5876	1054	1202	20			
1	A	788	Total	C	H	N	O	S	0	1	0
			12130	3940	5897	1061	1212	20			
1	C	778	Total	C	H	N	O	S	0	1	0
			12038	3901	5873	1050	1195	19			
1	D	776	Total	C	H	N	O	S	0	1	0
			11971	3881	5837	1045	1188	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ALA	ASP	engineered mutation	UNP A0A161XU12
A	678	ALA	ASP	engineered mutation	UNP A0A161XU12
C	678	ALA	ASP	engineered mutation	UNP A0A161XU12
D	678	ALA	ASP	engineered mutation	UNP A0A161XU12

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
5	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
5	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
5	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

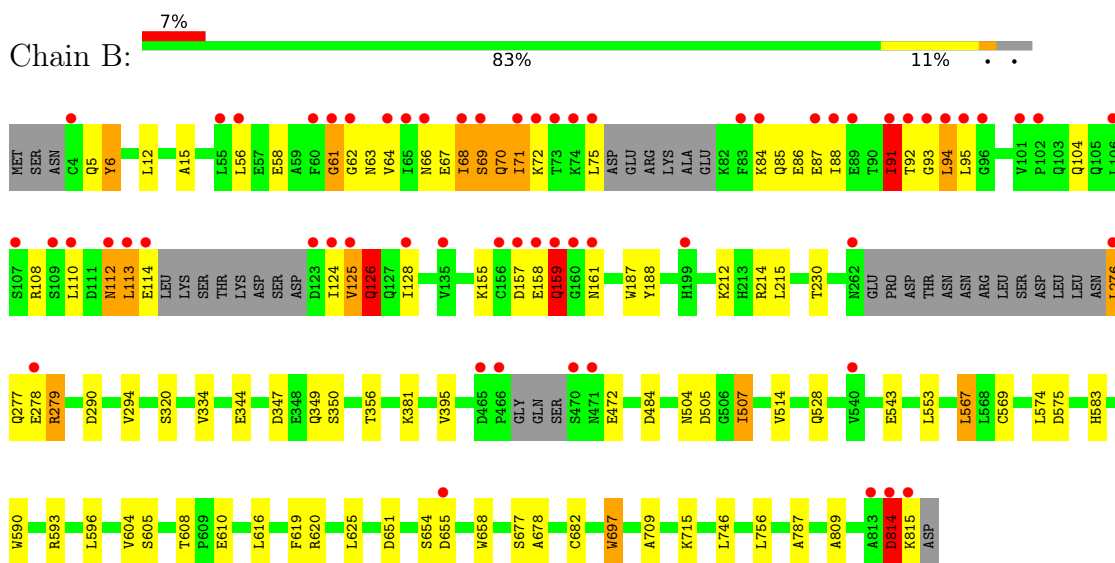
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	589	Total	O	0	0
			589	589		
6	A	532	Total	O	0	0
			532	532		
6	C	564	Total	O	0	0
			564	564		
6	D	480	Total	O	0	0
			480	480		

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.

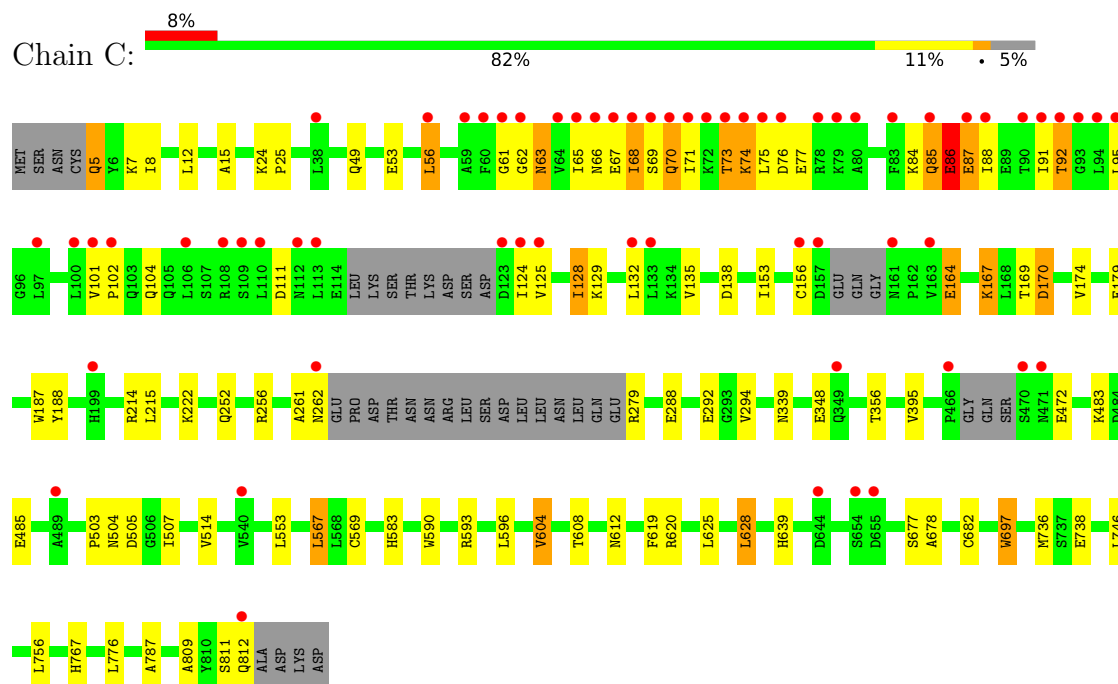
• Molecule 1: Uncharacterized protein



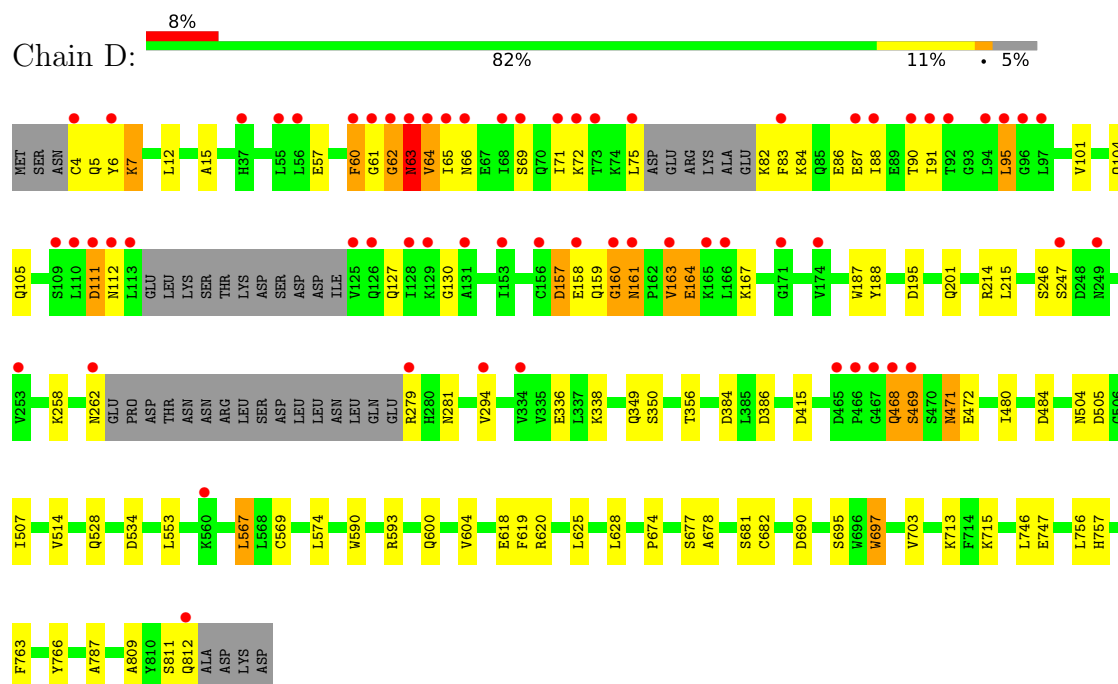
• Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.68Å 93.35Å 187.85Å 90.00° 94.95° 90.00°	Depositor
Resolution (Å)	48.29 – 1.96 48.29 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.29-1.96) 99.1 (48.29-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.175 , 0.209 0.177 , 0.210	Depositor DCC
R_{free} test set	2004 reflections (0.73%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	50448	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, TRQ, PEG

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	0.22	1/6365 (0.0%)	0.46	4/8662 (0.0%)
1	B	0.61	8/6328 (0.1%)	0.69	12/8614 (0.1%)
1	C	0.22	0/6296	0.46	0/8570
1	D	0.19	0/6266	0.42	2/8530 (0.0%)
All	All	0.36	9/25255 (0.0%)	0.52	18/34376 (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	A	0	3
1	B	0	2
1	C	0	1
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	TYR	CD1-CE1	25.84	2.16	1.38
1	B	6	TYR	CD2-CE2	25.56	2.15	1.38
1	B	6	TYR	CE1-CZ	-12.96	1.07	1.38
1	B	6	TYR	CE2-CZ	-12.77	1.07	1.38
1	B	6	TYR	CG-CD1	-10.90	1.16	1.39
1	B	6	TYR	CG-CD2	-10.79	1.16	1.39
1	B	583	HIS	CG-ND1	-8.73	1.28	1.38
1	B	583	HIS	CD2-NE2	-8.43	1.28	1.37
1	A	225	ASN	C-O	5.74	1.26	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	TYR	CD1-CG-CD2	-24.95	80.68	118.10
1	B	6	TYR	CE1-CZ-CE2	-21.91	76.48	120.30
1	B	6	TYR	CG-CD1-CE1	-15.58	97.83	121.20
1	B	6	TYR	CG-CD2-CE2	-15.51	97.94	121.20
1	B	6	TYR	CZ-CE2-CD2	-10.51	100.69	119.60
1	B	6	TYR	CD1-CE1-CZ	-10.48	100.73	119.60
1	B	6	TYR	CB-CG-CD1	10.40	136.41	120.80
1	B	6	TYR	CB-CG-CD2	10.33	136.29	120.80
1	B	110	LEU	CA-C-N	8.23	131.63	120.44
1	B	110	LEU	C-N-CA	8.23	131.63	120.44
1	B	6	TYR	OH-CZ-CE2	7.37	142.02	119.90
1	B	6	TYR	CE1-CZ-OH	7.20	141.49	119.90
1	D	160	GLY	CA-C-N	5.79	132.13	121.70
1	D	160	GLY	C-N-CA	5.79	132.13	121.70
1	A	465	ASP	CA-C-N	-5.16	113.40	119.84
1	A	465	ASP	C-N-CA	-5.16	113.40	119.84
1	A	464	ASP	CA-C-N	-5.04	117.39	122.83
1	A	464	ASP	C-N-CA	-5.04	117.39	122.83

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ASN	Peptide
1	A	469	SER	Peptide
1	A	94	LEU	Peptide
1	B	6	TYR	Sidechain
1	B	91	ILE	Peptide
1	C	77	GLU	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	6233	5897	6007	69	0
1	B	6197	5876	5973	54	0
1	C	6165	5873	5944	64	0
1	D	6134	5837	5913	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	7	10	10	2	0
5	A	10	10	4	4	0
5	C	5	5	2	4	0
5	D	5	5	2	3	0
6	A	532	0	0	16	0
6	B	589	0	0	7	0
6	C	564	0	0	13	0
6	D	480	0	0	16	0
All	All	26935	23513	23855	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 5.

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)
1:B:814:ASP:CB	1:B:815:LYS:HA	1.87	1.03
1:B:814:ASP:HB3	1:B:815:LYS:HA	1.37	1.03
1:D:766:TYR:OH	5:D:902:GLY:OXT	1.79	1.00
1:B:279:ARG:NH2	6:B:1001:HOH:O	2.02	0.92
1:A:80:ALA:HB1	1:A:82:LYS:H	1.35	0.90
1:B:814:ASP:HB3	1:B:815:LYS:CA	2.05	0.87
1:B:709:ALA:HB2	1:B:815:LYS:H	1.40	0.86
1:A:80:ALA:HA	1:A:81:GLU:CB	2.05	0.85
1:B:214:ARG:NH1	1:B:472:GLU:OE1	2.09	0.84
1:A:80:ALA:HA	1:A:81:GLU:HB3	1.58	0.84
1:D:690:ASP:OD2	6:D:1001:HOH:O	1.97	0.83
1:D:82:LYS:NZ	1:D:111:ASP:O	2.09	0.83
1:A:320:SER:OG	6:A:1001:HOH:O	2.00	0.80
1:B:678:ALA:HB1	6:B:1124:HOH:O	1.82	0.80
1:A:4:CYS:SG	6:A:1431:HOH:O	2.38	0.79
1:A:80:ALA:CA	1:A:81:GLU:HB3	2.13	0.79
1:C:485:GLU:OE1	6:C:1001:HOH:O	2.01	0.79
1:B:814:ASP:CG	1:B:815:LYS:HA	2.08	0.79
1:D:811:SER:O	6:D:1002:HOH:O	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:GLN:OE1	6:A:1002:HOH:O	2.01	0.78
1:A:471:ASN:ND2	6:A:1004:HOH:O	2.16	0.78
1:C:68:ILE:HG23	1:C:124:ILE:HD11	1.66	0.78
1:C:124:ILE:O	1:C:128:ILE:HG23	1.85	0.77
1:C:288:GLU:OE2	6:C:1002:HOH:O	2.03	0.75
1:D:160:GLY:H	1:D:161:ASN:HB2	1.51	0.75
1:D:214:ARG:NH1	1:D:472:GLU:OE2	2.20	0.74
1:B:92:THR:O	1:B:94:LEU:N	2.20	0.74
1:C:214:ARG:NH1	1:C:472:GLU:OE1	2.20	0.74
1:B:320:SER:OG	6:B:1002:HOH:O	2.07	0.73
1:C:612:ASN:ND2	6:C:1008:HOH:O	2.22	0.73
1:C:483:LYS:NZ	6:C:1006:HOH:O	2.21	0.73
1:A:157:ASP:OD1	6:A:1003:HOH:O	2.06	0.72
1:D:157:ASP:OD2	1:D:160:GLY:N	2.23	0.72
1:B:484:ASP:OD1	6:B:1003:HOH:O	2.08	0.72
1:A:767:HIS:NE2	5:A:904:GLY:OXT	2.23	0.71
1:A:80:ALA:CB	1:A:81:GLU:HB3	2.21	0.71
1:C:73:THR:O	1:C:75:LEU:N	2.23	0.71
1:C:339:ASN:OD1	6:C:1003:HOH:O	2.09	0.70
1:D:201:GLN:NE2	6:D:1008:HOH:O	2.23	0.70
1:A:620:ARG:NH2	6:A:1006:HOH:O	2.18	0.70
1:B:610:GLU:OE1	6:B:1004:HOH:O	2.10	0.69
1:D:415:ASP:O	6:D:1003:HOH:O	2.09	0.69
1:A:812:GLN:N	6:A:1007:HOH:O	2.22	0.69
1:D:160:GLY:N	1:D:161:ASN:HB2	2.08	0.68
1:C:8:ILE:O	1:C:620:ARG:NH2	2.27	0.67
5:C:902:GLY:N	1:D:697:TRQ:O6	2.28	0.67
1:B:61:GLY:HA2	1:B:63:ASN:N	2.10	0.67
1:D:349:GLN:OE1	1:D:600:GLN:NE2	2.28	0.67
1:B:68:ILE:O	1:B:70:GLN:N	2.28	0.66
1:B:277:GLN:OE1	6:B:1005:HOH:O	2.13	0.66
1:D:63:ASN:O	1:D:65:ILE:N	2.29	0.66
1:B:61:GLY:HA2	1:B:64:VAL:H	1.59	0.66
1:C:485:GLU:OE2	6:C:1004:HOH:O	2.12	0.66
1:D:384:ASP:OD2	6:D:1004:HOH:O	2.13	0.66
1:D:682:CYS:SG	1:D:697:TRQ:HB3	2.36	0.65
1:A:83:PHE:O	1:A:84:LYS:HB2	1.95	0.65
1:C:128:ILE:HG13	1:C:129:LYS:N	2.12	0.65
1:A:201:GLN:NE2	6:A:1008:HOH:O	2.29	0.64
5:A:904:GLY:N	6:A:1010:HOH:O	2.29	0.64
1:C:111:ASP:OD1	6:C:1005:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ILE:CG2	1:C:124:ILE:HD11	2.28	0.64
1:D:484:ASP:OD1	6:D:1005:HOH:O	2.15	0.64
1:A:678:ALA:HB1	6:A:1074:HOH:O	1.97	0.64
1:C:61:GLY:O	1:C:63:ASN:N	2.31	0.64
1:B:709:ALA:CB	1:B:815:LYS:HG2	2.29	0.63
1:A:80:ALA:HB1	1:A:81:GLU:HB3	1.82	0.61
1:C:73:THR:O	1:C:76:ASP:N	2.29	0.61
1:D:60:PHE:O	1:D:62:GLY:N	2.31	0.61
1:C:5:GLN:N	6:C:1012:HOH:O	2.33	0.60
1:C:678:ALA:HB1	6:C:1023:HOH:O	2.01	0.60
1:B:697:TRQ:O6	5:A:904:GLY:N	2.34	0.60
1:C:66:ASN:OD1	1:C:67:GLU:N	2.34	0.59
1:C:682:CYS:SG	1:C:697:TRQ:HB3	2.42	0.59
1:C:179:GLU:HB2	1:C:628:LEU:HD22	1.83	0.59
1:A:8:ILE:O	1:A:620:ARG:NH2	2.36	0.59
1:B:619:PHE:O	1:B:620:ARG:HD2	2.03	0.59
1:B:682:CYS:SG	1:B:697:TRQ:HB3	2.43	0.59
1:A:682:CYS:SG	1:A:697:TRQ:HB3	2.43	0.59
1:D:747:GLU:OE2	6:D:1006:HOH:O	2.16	0.58
1:D:471:ASN:ND2	6:D:1013:HOH:O	2.35	0.58
1:A:620:ARG:NH1	6:A:1006:HOH:O	2.31	0.58
1:A:24:LYS:HE3	4:A:902:PEG:H42	1.85	0.57
1:A:812:GLN:N	6:A:1019:HOH:O	2.37	0.57
1:B:63:ASN:OD1	1:B:66:ASN:ND2	2.38	0.57
1:A:80:ALA:HA	1:A:81:GLU:HB2	1.87	0.57
1:D:620:ARG:NH1	6:D:1010:HOH:O	2.36	0.57
1:A:600:GLN:NE2	6:A:1011:HOH:O	2.30	0.57
1:B:567:LEU:HD23	1:B:604:VAL:HG21	1.88	0.55
1:C:128:ILE:HD12	1:C:132:LEU:HD11	1.88	0.55
1:D:246:SER:OG	6:D:1007:HOH:O	2.18	0.55
1:D:468:GLN:O	1:D:469:SER:CB	2.54	0.55
1:B:61:GLY:HA2	1:B:62:GLY:C	2.32	0.55
1:B:276:LEU:HG	1:C:138:ASP:HB3	1.88	0.55
1:D:15:ALA:O	1:D:356:THR:HA	2.06	0.55
1:B:158:GLU:O	1:B:159:GLN:HB2	2.07	0.54
1:C:590:TRP:O	1:C:593:ARG:HB2	2.06	0.54
1:A:349:GLN:O	1:A:620:ARG:HD2	2.07	0.54
1:C:767:HIS:NE2	5:C:902:GLY:OXT	2.40	0.54
1:B:15:ALA:O	1:B:356:THR:HA	2.08	0.54
1:B:567:LEU:CD2	1:B:604:VAL:HG21	2.37	0.53
1:A:15:ALA:O	1:A:356:THR:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLU:OE2	1:A:620:ARG:NH1	2.42	0.53
1:A:766:TYR:OH	5:A:904:GLY:O	2.25	0.53
1:D:111:ASP:O	1:D:111:ASP:CG	2.51	0.53
1:A:76:ASP:O	1:A:79:LYS:HE3	2.08	0.53
1:D:86:GLU:O	1:D:90:THR:OG1	2.19	0.52
1:A:469:SER:HA	1:A:471:ASN:OD1	2.08	0.52
1:C:252:GLN:NE2	1:C:288:GLU:OE2	2.43	0.52
1:D:63:ASN:OD1	1:D:63:ASN:N	2.42	0.52
1:D:678:ALA:HB1	6:D:1025:HOH:O	2.09	0.52
1:A:169:THR:OG1	1:A:172:ASP:OD2	2.26	0.51
1:B:125:VAL:O	1:B:126:GLN:NE2	2.38	0.51
1:B:68:ILE:O	1:B:71:ILE:HD13	2.09	0.51
1:C:222:LYS:NZ	6:C:1022:HOH:O	2.44	0.51
1:D:620:ARG:NH2	6:D:1010:HOH:O	2.39	0.51
1:B:507:ILE:HD12	1:A:766:TYR:CD1	2.46	0.51
1:A:795:GLU:OE2	6:A:1005:HOH:O	2.18	0.51
5:C:902:GLY:HA2	1:D:681[B]:SER:O	2.11	0.50
1:A:542:LYS:NZ	6:A:1029:HOH:O	2.41	0.50
1:C:124:ILE:HD12	1:C:125:VAL:N	2.27	0.50
1:D:567:LEU:CD2	1:D:604:VAL:HG21	2.42	0.50
1:C:567:LEU:CD2	1:C:604:VAL:HG21	2.41	0.50
1:D:7:LYS:NZ	6:D:1027:HOH:O	2.45	0.49
1:D:82:LYS:HG3	1:D:83:PHE:H	1.77	0.49
1:B:85:GLN:O	1:B:88:ILE:N	2.46	0.49
1:C:15:ALA:O	1:C:356:THR:HA	2.12	0.49
1:A:567:LEU:CD2	1:A:604:VAL:HG21	2.43	0.49
1:D:619:PHE:O	1:D:620:ARG:HG2	2.12	0.49
1:A:80:ALA:HB1	1:A:82:LYS:N	2.17	0.49
1:A:463:VAL:CG1	1:A:466:PRO:HB3	2.42	0.49
1:A:469:SER:O	1:A:470:SER:OG	2.31	0.49
1:C:261:ALA:O	1:C:279:ARG:NH2	2.45	0.49
1:C:787:ALA:HB1	1:C:809:ALA:HB1	1.94	0.48
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.95	0.48
1:C:101:VAL:HG13	1:C:102:PRO:HD2	1.96	0.48
1:B:68:ILE:O	1:B:71:ILE:N	2.34	0.48
1:A:348:GLU:O	1:A:620:ARG:HD3	2.14	0.48
1:A:339:ASN:OD1	1:A:339:ASN:N	2.43	0.48
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.96	0.48
1:D:468:GLN:O	1:D:469:SER:HB3	2.13	0.48
1:B:187:TRP:CG	1:B:188:TYR:H	2.32	0.48
1:D:160:GLY:CA	1:D:161:ASN:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:PRO:HD2	1:D:677:SER:HG	1.79	0.47
1:C:256:ARG:NH1	6:C:1015:HOH:O	2.38	0.47
1:C:261:ALA:O	1:C:262:ASN:HB2	2.13	0.47
1:D:349:GLN:HA	1:D:620:ARG:HD3	1.96	0.47
1:B:87:GLU:O	1:B:91:ILE:HG23	2.15	0.47
1:C:124:ILE:HD12	1:C:124:ILE:C	2.39	0.47
1:B:590:TRP:O	1:B:593:ARG:HG2	2.15	0.47
1:B:787:ALA:HB1	1:B:809:ALA:HB1	1.96	0.47
1:C:187:TRP:CG	1:C:188:TYR:H	2.33	0.47
1:D:677:SER:HB2	6:D:1249:HOH:O	2.15	0.47
1:D:811:SER:O	1:D:812:GLN:HB2	2.13	0.47
1:A:187:TRP:CG	1:A:188:TYR:H	2.33	0.47
1:A:503:PRO:HB3	1:A:507:ILE:HD12	1.97	0.47
1:B:709:ALA:HB2	1:B:815:LYS:HG2	1.97	0.47
1:A:250:ASN:HA	1:A:289:CYS:O	2.14	0.47
1:D:187:TRP:CG	1:D:188:TYR:H	2.33	0.46
1:B:112:ASN:N	1:B:112:ASN:OD1	2.49	0.46
1:A:172:ASP:OD1	1:A:338:LYS:N	2.47	0.46
1:A:469:SER:O	1:A:470:SER:CB	2.63	0.46
1:A:6:TYR:O	1:A:350:SER:OG	2.33	0.46
1:C:593:ARG:HD3	6:C:1313:HOH:O	2.15	0.46
1:D:64:VAL:HG12	1:D:65:ILE:N	2.29	0.46
1:B:68:ILE:O	1:B:69:SER:C	2.58	0.46
1:B:68:ILE:C	1:B:70:GLN:N	2.74	0.46
1:D:5:GLN:HG2	1:D:6:TYR:H	1.81	0.46
1:A:156:CYS:HA	1:A:161:ASN:O	2.16	0.46
1:A:290:ASP:HB3	4:A:902:PEG:O2	2.16	0.46
1:A:76:ASP:O	1:A:78:ARG:N	2.49	0.46
1:A:620:ARG:CZ	6:A:1006:HOH:O	2.56	0.46
1:C:811:SER:O	1:C:812:GLN:HB2	2.16	0.45
1:A:590:TRP:O	1:A:593:ARG:HG3	2.17	0.45
1:C:169:THR:O	1:C:170:ASP:C	2.59	0.45
1:D:95:LEU:O	1:D:95:LEU:HD23	2.16	0.45
1:A:79:LYS:HA	1:A:79:LYS:HD3	1.84	0.45
1:D:157:ASP:O	1:D:160:GLY:HA3	2.17	0.45
1:C:88:ILE:O	1:C:92:THR:HG23	2.17	0.45
1:D:195:ASP:OD2	1:D:593:ARG:HD2	2.16	0.45
1:D:713:LYS:NZ	6:D:1037:HOH:O	2.49	0.45
1:D:69:SER:HA	1:D:72:LYS:HB2	1.98	0.45
1:D:82:LYS:HG3	1:D:83:PHE:N	2.32	0.44
1:C:503:PRO:HB3	1:C:507:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:LEU:HD23	1:D:604:VAL:HG21	1.99	0.44
1:B:814:ASP:OD2	6:B:1006:HOH:O	2.21	0.44
1:B:504:ASN:CG	1:B:505:ASP:H	2.26	0.44
1:A:464:ASP:O	1:A:465:ASP:C	2.58	0.44
1:A:811:SER:C	1:A:813:ALA:H	2.25	0.44
1:C:68:ILE:HG21	1:C:125:VAL:HG22	2.00	0.44
5:C:902:GLY:HA2	1:D:681[A]:SER:O	2.18	0.44
1:D:386:ASP:OD1	1:D:386:ASP:N	2.50	0.44
1:C:84:LYS:O	1:C:88:ILE:HG12	2.17	0.44
1:D:62:GLY:O	1:D:63:ASN:C	2.60	0.44
1:A:195:ASP:OD2	1:A:593:ARG:HD2	2.18	0.44
1:C:85:GLN:C	1:C:86:GLU:HG3	2.43	0.44
1:A:500:PRO:HB2	1:A:502:TYR:CE2	2.53	0.43
1:D:7:LYS:HG3	1:D:350:SER:HA	1.99	0.43
1:A:71:ILE:HG12	1:A:75:LEU:CD2	2.48	0.43
1:C:84:LYS:O	1:C:87:GLU:HB2	2.18	0.43
1:A:514:VAL:HG12	1:A:514:VAL:O	2.18	0.43
1:D:682:CYS:HB2	1:D:697:TRQ:HZ3	1.77	0.43
1:C:86:GLU:HA	1:C:88:ILE:N	2.34	0.43
1:C:68:ILE:O	1:C:71:ILE:HB	2.19	0.43
1:D:528:GLN:HG3	6:D:1092:HOH:O	2.17	0.43
1:C:7:LYS:HD3	1:C:156:CYS:SG	2.59	0.43
1:D:618:GLU:OE2	1:D:620:ARG:NH1	2.52	0.43
1:A:45:TYR:CD2	1:A:790:MET:HG2	2.53	0.43
1:C:514:VAL:HG12	1:C:514:VAL:O	2.19	0.43
1:D:504:ASN:CG	1:D:505:ASP:H	2.27	0.43
1:D:163:VAL:O	1:D:164:GLU:O	2.37	0.42
1:B:709:ALA:HB1	1:B:815:LYS:HG2	2.01	0.42
1:A:504:ASN:CG	1:A:505:ASP:H	2.27	0.42
1:B:514:VAL:HG12	1:B:514:VAL:O	2.20	0.42
1:B:604:VAL:HG22	1:B:616:LEU:O	2.19	0.42
1:A:509:TYR:CD1	1:C:639:HIS:HB3	2.54	0.42
1:A:386:ASP:OD1	1:A:386:ASP:N	2.52	0.42
1:C:73:THR:C	1:C:75:LEU:N	2.78	0.42
1:D:590:TRP:O	1:D:593:ARG:CG	2.68	0.42
1:B:113:LEU:N	1:B:113:LEU:HD23	2.35	0.42
1:A:179:GLU:HB2	1:A:628:LEU:HD22	2.01	0.42
1:C:86:GLU:O	1:C:86:GLU:OE2	2.38	0.42
1:C:504:ASN:CG	1:C:505:ASP:H	2.28	0.42
1:D:91:ILE:O	1:D:95:LEU:HD22	2.19	0.42
1:B:604:VAL:HG23	1:B:605:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:VAL:HG12	1:D:514:VAL:O	2.20	0.41
1:B:84:LYS:HB2	1:B:87:GLU:HB2	2.02	0.41
1:C:70:GLN:O	1:C:74:LYS:HD3	2.20	0.41
1:C:619:PHE:O	1:C:620:ARG:HD2	2.20	0.41
1:D:349:GLN:O	1:D:620:ARG:HD2	2.19	0.41
1:B:157:ASP:HB2	1:B:161:ASN:H	1.86	0.41
1:C:583:HIS:ND1	5:D:902:GLY:OXT	2.53	0.41
1:D:262:ASN:HB2	1:D:279:ARG:HH12	1.86	0.41
1:C:167:LYS:NZ	1:C:292:GLU:OE1	2.48	0.41
1:D:695:SER:HB2	1:D:703:VAL:HG21	2.02	0.41
1:A:757:HIS:HA	1:A:763:PHE:CZ	2.56	0.41
1:C:69:SER:C	1:C:71:ILE:H	2.28	0.41
1:C:583:HIS:O	5:D:902:GLY:HA2	2.20	0.41
1:D:88:ILE:HD11	1:D:111:ASP:HB2	2.02	0.41
1:B:655:ASP:O	1:B:658:TRP:HD1	2.03	0.41
1:A:250:ASN:OD1	1:A:250:ASN:C	2.64	0.41
1:A:738:GLU:O	1:A:742:GLU:HG2	2.21	0.41
1:C:24:LYS:HB2	1:C:25:PRO:HD3	2.03	0.41
1:D:258:LYS:HE2	1:D:281:ASN:OD1	2.21	0.41
1:D:480:ILE:HG21	1:D:507:ILE:HD11	2.02	0.41
1:C:53:GLU:O	1:C:56:LEU:HD22	2.20	0.41
1:B:290:ASP:OD2	1:B:294:VAL:CG1	2.69	0.40
1:B:682:CYS:HB2	1:B:697:TRQ:HZ3	1.81	0.40
1:A:608:THR:O	1:A:609:PRO:C	2.65	0.40
1:C:348:GLU:O	1:C:620:ARG:HG2	2.22	0.40
1:C:348:GLU:OE2	6:C:1007:HOH:O	2.22	0.40
1:B:347:ASP:OD1	1:B:350:SER:OG	2.30	0.40
1:B:651:ASP:HB3	1:B:654:SER:HB2	2.03	0.40
1:D:757:HIS:HA	1:D:763:PHE:CZ	2.56	0.40
1:A:258:LYS:HD3	1:A:279:ARG:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	780/816 (96%)	739 (95%)	32 (4%)	9 (1%)	10	4
1	B	773/816 (95%)	740 (96%)	24 (3%)	9 (1%)	10	4
1	C	768/816 (94%)	737 (96%)	24 (3%)	7 (1%)	14	6
1	D	768/816 (94%)	730 (95%)	28 (4%)	10 (1%)	9	3
All	All	3089/3264 (95%)	2946 (95%)	108 (4%)	35 (1%)	11	4

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	159	GLN
1	A	81	GLU
1	A	84	LYS
1	C	62	GLY
1	C	74	LYS
1	B	61	GLY
1	B	93	GLY
1	B	814	ASP
1	A	78	ARG
1	A	469	SER
1	A	470	SER
1	C	73	THR
1	D	61	GLY
1	D	62	GLY
1	D	63	ASN
1	D	64	VAL
1	D	158	GLU
1	D	469	SER
1	A	62	GLY
1	A	94	LEU
1	C	170	ASP
1	D	60	PHE
1	D	164	GLU
1	A	279	ARG
1	C	87	GLU
1	A	77	GLU
1	C	164	GLU
1	D	161	ASN
1	B	126	GLN

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Mol	Chain	Res	Type
1	B	230	THR
1	C	86	GLU
1	B	68	ILE
1	B	125	VAL
1	D	130	GLY

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	684/710 (96%)	641 (94%)	43 (6%)	16	6
1	B	680/710 (96%)	631 (93%)	49 (7%)	13	4
1	C	676/710 (95%)	639 (94%)	37 (6%)	19	8
1	D	673/710 (95%)	635 (94%)	38 (6%)	19	8
All	All	2713/2840 (96%)	2546 (94%)	167 (6%)	16	6

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	GLN
1	B	12	LEU
1	B	56	LEU
1	B	58	GLU
1	B	67	GLU
1	B	70	GLN
1	B	71	ILE
1	B	72	LYS
1	B	75	LEU
1	B	86	GLU
1	B	91	ILE
1	B	94	LEU
1	B	95	LEU
1	B	104	GLN
1	B	108	ARG
1	B	112	ASN

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Mol	Chain	Res	Type
1	B	113	LEU
1	B	114	GLU
1	B	124	ILE
1	B	126	GLN
1	B	128	ILE
1	B	155	LYS
1	B	159	GLN
1	B	212	LYS
1	B	215	LEU
1	B	276	LEU
1	B	278	GLU
1	B	279	ARG
1	B	334	VAL
1	B	344	GLU
1	B	349	GLN
1	B	381	LYS
1	B	395	VAL
1	B	507	ILE
1	B	528	GLN
1	B	543	GLU
1	B	553	LEU
1	B	567	LEU
1	B	569	CYS
1	B	574	LEU
1	B	575	ASP
1	B	596	LEU
1	B	608	THR
1	B	625	LEU
1	B	677	SER
1	B	715	LYS
1	B	746	LEU
1	B	756	LEU
1	B	814	ASP
1	A	12	LEU
1	A	58	GLU
1	A	64	VAL
1	A	66	ASN
1	A	69	SER
1	A	70	GLN
1	A	71	ILE
1	A	72	LYS
1	A	73	THR

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	84	LYS
1	A	95	LEU
1	A	111	ASP
1	A	114	GLU
1	A	116	LYS
1	A	127	GLN
1	A	153	ILE
1	A	164	GLU
1	A	173	LYS
1	A	247	SER
1	A	262	ASN
1	A	278	GLU
1	A	279	ARG
1	A	294	VAL
1	A	339	ASN
1	A	381	LYS
1	A	424	GLU
1	A	465	ASP
1	A	534	ASP
1	A	553	LEU
1	A	560	LYS
1	A	569	CYS
1	A	575	ASP
1	A	593	ARG
1	A	608	THR
1	A	620	ARG
1	A	628	LEU
1	A	677	SER
1	A	738	GLU
1	A	746	LEU
1	A	756	LEU
1	A	796	ASN
1	A	812	GLN
1	C	5	GLN
1	C	12	LEU
1	C	49	GLN
1	C	56	LEU
1	C	63	ASN
1	C	65	ILE
1	C	68	ILE
1	C	70	GLN

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	86	GLU
1	C	91	ILE
1	C	92	THR
1	C	95	LEU
1	C	104	GLN
1	C	128	ILE
1	C	135	VAL
1	C	153	ILE
1	C	164	GLU
1	C	167	LYS
1	C	174	VAL
1	C	215	LEU
1	C	294	VAL
1	C	395	VAL
1	C	553	LEU
1	C	567	LEU
1	C	569	CYS
1	C	596	LEU
1	C	604	VAL
1	C	608	THR
1	C	625	LEU
1	C	628	LEU
1	C	677	SER
1	C	736	MET
1	C	738	GLU
1	C	746	LEU
1	C	756	LEU
1	C	776	LEU
1	D	4	CYS
1	D	7	LYS
1	D	12	LEU
1	D	57	GLU
1	D	63	ASN
1	D	66	ASN
1	D	71	ILE
1	D	75	LEU
1	D	84	LYS
1	D	87	GLU
1	D	95	LEU
1	D	101	VAL
1	D	104	GLN

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Mol	Chain	Res	Type
1	D	105	GLN
1	D	111	ASP
1	D	112	ASN
1	D	127	GLN
1	D	157	ASP
1	D	159	GLN
1	D	163	VAL
1	D	167	LYS
1	D	215	LEU
1	D	247	SER
1	D	294	VAL
1	D	336	GLU
1	D	338	LYS
1	D	468	GLN
1	D	471	ASN
1	D	534	ASP
1	D	553	LEU
1	D	567	LEU
1	D	569	CYS
1	D	574	LEU
1	D	625	LEU
1	D	628	LEU
1	D	715	LYS
1	D	746	LEU
1	D	756	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	66	ASN
1	B	433	GLN
1	B	451	GLN
1	B	471	ASN
1	B	525	GLN
1	B	632	ASN
1	B	635	GLN
1	B	785	ASN
1	A	70	GLN
1	A	236	GLN
1	A	284	GLN
1	A	451	GLN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	683	GLN
1	C	5	GLN
1	C	103	GLN
1	C	199	HIS
1	C	284	GLN
1	C	346	GLN
1	C	410	GLN
1	C	433	GLN
1	C	451	GLN
1	C	525	GLN
1	C	653	ASN
1	C	683	GLN
1	C	730	HIS
1	D	66	ASN
1	D	99	HIS
1	D	213	HIS
1	D	236	GLN
1	D	471	ASN
1	D	600	GLN
1	D	751	GLN
1	D	804	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	TRQ	D	697	1	16,17,18	1.13	1 (6%)	16,24,26	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TRQ	C	697	1	16,17,18	1.20	1 (6%)	16,24,26	0.97	1 (6%)
1	TRQ	A	697	1	16,17,18	1.18	1 (6%)	16,24,26	1.00	1 (6%)
1	TRQ	B	697	1	16,17,18	1.10	1 (6%)	16,24,26	1.01	1 (6%)

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
1	TRQ	D	697	1	-	2/5/19/21	0/2/2/2
1	TRQ	C	697	1	-	2/5/19/21	0/2/2/2
1	TRQ	A	697	1	-	2/5/19/21	0/2/2/2
1	TRQ	B	697	1	-	1/5/19/21	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TRQ	CD1-CG	2.85	1.42	1.38
1	A	697	TRQ	CD1-CG	2.80	1.42	1.38
1	C	697	TRQ	CD1-CG	2.65	1.42	1.38
1	B	697	TRQ	CD1-CG	2.50	1.41	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	697	TRQ	O7-CZ2-CH2	2.96	122.16	118.39
1	B	697	TRQ	O7-CZ2-CH2	2.80	121.96	118.39
1	A	697	TRQ	O7-CZ2-CH2	2.76	121.91	118.39
1	D	697	TRQ	O7-CZ2-CH2	2.37	121.42	118.39

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	697	TRQ	CA-CB-CG-CD2
1	C	697	TRQ	CA-CB-CG-CD2
1	D	697	TRQ	CA-CB-CG-CD2
1	A	697	TRQ	CA-CB-CG-CD1
1	D	697	TRQ	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	C	697	TRQ	CA-CB-CG-CD1
1	B	697	TRQ	CA-CB-CG-CD1

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	697	TRQ	3	0
1	C	697	TRQ	1	0
1	A	697	TRQ	1	0
1	B	697	TRQ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	GLY	A	904	-	4,4,4	1.28	1 (25%)	3,4,4	1.07	0
5	GLY	A	903	-	4,4,4	1.21	1 (25%)	3,4,4	1.29	0
4	PEG	A	902	-	6,6,6	0.55	0	5,5,5	0.59	0
5	GLY	D	902	-	4,4,4	1.13	1 (25%)	3,4,4	1.71	2 (66%)
5	GLY	C	902	-	4,4,4	1.13	1 (25%)	3,4,4	1.64	1 (33%)
3	SO4	C	903	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	B	902	-	4,4,4	0.21	0	6,6,6	0.18	0

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	GLY	A	904	-	-	2/2/2/2	-
5	GLY	A	903	-	-	0/2/2/2	-
4	PEG	A	902	-	-	3/4/4/4	-
5	GLY	D	902	-	-	0/2/2/2	-
5	GLY	C	902	-	-	0/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	GLY	OXT-C	-2.38	1.23	1.30
5	A	903	GLY	OXT-C	-2.28	1.23	1.30
5	C	902	GLY	OXT-C	-2.18	1.23	1.30
5	D	902	GLY	OXT-C	-2.18	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	902	GLY	OXT-C-O	-2.12	117.87	123.33
5	D	902	GLY	OXT-C-CA	2.09	121.68	113.38
5	D	902	GLY	OXT-C-O	-2.04	118.08	123.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	PEG	O1-C1-C2-O2
4	A	902	PEG	O2-C3-C4-O4
4	A	902	PEG	C4-C3-O2-C2
5	A	904	GLY	OXT-C-CA-N
5	A	904	GLY	O-C-CA-N

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	904	GLY	4	0
4	A	902	PEG	2	0
5	D	902	GLY	3	0
5	C	902	GLY	4	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 [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	787/816 (96%)	0.23	54 (6%)	23	26	12, 37, 96, 136	1 (0%)
1	B	781/816 (95%)	0.09	60 (7%)	19	22	18, 31, 100, 152	2 (0%)
1	C	777/816 (95%)	0.10	63 (8%)	18	21	17, 32, 110, 174	1 (0%)
1	D	775/816 (94%)	0.29	62 (8%)	18	21	13, 40, 105, 173	1 (0%)
All	All	3120/3264 (95%)	0.18	239 (7%)	19	22	12, 34, 103, 174	5 (0%)

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	813	ALA	8.4
1	D	83	PHE	5.9
1	B	540[A]	VAL	5.6
1	D	125	VAL	5.6
1	A	262	ASN	5.4
1	C	94	LEU	5.3
1	D	68	ILE	5.3
1	D	75	LEU	5.1
1	C	125	VAL	5.1
1	B	470	SER	5.1
1	B	158	GLU	5.0
1	D	91	ILE	4.9
1	A	466	PRO	4.8
1	C	124	ILE	4.8
1	A	80	ALA	4.7
1	B	73	THR	4.7
1	D	158	GLU	4.7
1	B	61	GLY	4.6
1	C	64	VAL	4.6
1	C	68	ILE	4.6
1	A	465	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	83	PHE	4.6
1	B	83	PHE	4.5
1	B	75	LEU	4.5
1	B	110	LEU	4.5
1	A	115	LEU	4.4
1	C	88	ILE	4.4
1	A	121	SER	4.4
1	D	73	THR	4.2
1	C	90	THR	4.1
1	A	95	LEU	4.1
1	B	4	CYS	3.9
1	B	814	ASP	3.9
1	B	124	ILE	3.9
1	B	62	GLY	3.9
1	D	467	GLY	3.8
1	B	91	ILE	3.8
1	D	88	ILE	3.8
1	C	101	VAL	3.8
1	A	467	GLY	3.7
1	D	94	LEU	3.7
1	D	113	LEU	3.7
1	C	65	ILE	3.7
1	B	276	LEU	3.7
1	A	113	LEU	3.7
1	D	110	LEU	3.7
1	A	75	LEU	3.6
1	A	469	SER	3.6
1	B	71	ILE	3.6
1	D	65	ILE	3.6
1	C	95	LEU	3.6
1	C	61	GLY	3.6
1	C	106	LEU	3.6
1	C	163	VAL	3.6
1	D	163	VAL	3.6
1	C	60	PHE	3.6
1	A	4	CYS	3.5
1	C	71	ILE	3.5
1	D	71	ILE	3.5
1	B	125	VAL	3.5
1	D	262	ASN	3.4
1	D	64	VAL	3.4
1	D	466	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	65	ILE	3.4
1	C	56	LEU	3.4
1	C	75	LEU	3.4
1	C	102	PRO	3.4
1	C	157	ASP	3.3
1	B	113	LEU	3.3
1	D	56	LEU	3.3
1	B	160	GLY	3.3
1	B	68	ILE	3.3
1	C	110	LEU	3.3
1	C	812	GLN	3.3
1	D	111	ASP	3.3
1	D	61	GLY	3.3
1	A	468	GLN	3.3
1	C	655	ASP	3.3
1	D	469	SER	3.3
1	C	156	CYS	3.2
1	D	812	GLN	3.2
1	A	163	VAL	3.2
1	C	87	GLU	3.2
1	C	161	ASN	3.1
1	B	94	LEU	3.1
1	D	279	ARG	3.1
1	C	113	LEU	3.1
1	C	112	ASN	3.1
1	C	91	ILE	3.1
1	B	815	LYS	3.1
1	B	471	ASN	3.1
1	D	66	ASN	3.1
1	D	4	CYS	3.1
1	A	93	GLY	3.0
1	B	72	LYS	3.0
1	A	116	LYS	3.0
1	A	122	ASP	3.0
1	B	88	ILE	3.0
1	B	107	SER	2.9
1	B	655	ASP	2.9
1	A	73	THR	2.9
1	D	95	LEU	2.9
1	C	123	ASP	2.9
1	B	466	PRO	2.9
1	C	74	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	69	SER	2.9
1	A	83	PHE	2.9
1	C	80	ALA	2.9
1	C	489	ALA	2.9
1	C	62	GLY	2.9
1	B	262	ASN	2.8
1	B	159	GLN	2.8
1	B	64	VAL	2.8
1	C	466	PRO	2.8
1	A	157	ASP	2.8
1	B	128	ILE	2.8
1	C	97	LEU	2.8
1	D	128	ILE	2.8
1	B	813	ALA	2.7
1	A	812	GLN	2.7
1	B	156	CYS	2.7
1	B	199	HIS	2.7
1	A	94	LEU	2.7
1	A	334	VAL	2.7
1	D	160	GLY	2.7
1	C	76	ASP	2.7
1	D	465	ASP	2.7
1	B	109	SER	2.7
1	D	69	SER	2.7
1	D	63	ASN	2.7
1	C	199	HIS	2.7
1	B	123	ASP	2.7
1	A	37	HIS	2.7
1	A	96	GLY	2.6
1	D	171	GLY	2.6
1	D	112	ASN	2.6
1	B	95	LEU	2.6
1	D	156	CYS	2.6
1	C	100	LEU	2.6
1	B	56	LEU	2.5
1	A	170	ASP	2.5
1	B	74	LYS	2.5
1	C	262	ASN	2.5
1	C	109	SER	2.5
1	B	102	PRO	2.5
1	B	60	PHE	2.5
1	D	60	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	72	LYS	2.5
1	D	129	LYS	2.5
1	B	106	LEU	2.5
1	D	62	GLY	2.5
1	B	161	ASN	2.5
1	A	85	GLN	2.5
1	B	66	ASN	2.5
1	A	68	ILE	2.5
1	A	71	ILE	2.5
1	A	91	ILE	2.5
1	D	294	VAL	2.5
1	A	249	ASN	2.4
1	C	38	LEU	2.4
1	B	89	GLU	2.4
1	D	249	ASN	2.4
1	A	64	VAL	2.4
1	D	166	LEU	2.4
1	C	59	ALA	2.4
1	A	63	ASN	2.4
1	B	93	GLY	2.4
1	D	96	GLY	2.4
1	B	69	SER	2.4
1	D	97	LEU	2.3
1	A	65	ILE	2.3
1	A	88	ILE	2.3
1	A	110	LEU	2.3
1	C	133	LEU	2.3
1	C	92	THR	2.3
1	D	90	THR	2.3
1	A	471	ASN	2.3
1	C	66	ASN	2.3
1	D	161	ASN	2.3
1	D	153	ILE	2.3
1	C	72	LYS	2.3
1	A	470	SER	2.3
1	C	108	ARG	2.3
1	B	101	VAL	2.3
1	B	465	ASP	2.3
1	C	540	VAL	2.3
1	B	114	GLU	2.3
1	B	55	LEU	2.3
1	C	471	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	LYS	2.3
1	B	96	GLY	2.3
1	A	128	ILE	2.3
1	D	109	SER	2.3
1	A	156	CYS	2.3
1	A	78	ARG	2.2
1	B	278	GLU	2.2
1	D	6	TYR	2.2
1	D	131	ALA	2.2
1	C	654	SER	2.2
1	D	37	HIS	2.2
1	C	73	THR	2.2
1	D	92	THR	2.2
1	B	84	LYS	2.2
1	A	553	LEU	2.2
1	B	157	ASP	2.2
1	A	130	GLY	2.2
1	C	93	GLY	2.2
1	A	77	GLU	2.2
1	D	334	VAL	2.2
1	D	468	GLN	2.2
1	B	92	THR	2.2
1	C	644	ASP	2.2
1	A	166	LEU	2.2
1	A	489	ALA	2.2
1	B	87	GLU	2.1
1	A	81	GLU	2.1
1	C	70	GLN	2.1
1	C	85	GLN	2.1
1	C	67	GLU	2.1
1	A	342	THR	2.1
1	D	165	LYS	2.1
1	D	560	LYS	2.1
1	C	132	LEU	2.1
1	C	349	GLN	2.1
1	D	126	GLN	2.1
1	C	470	SER	2.1
1	B	112	ASN	2.1
1	A	104	GLN	2.1
1	D	55	LEU	2.1
1	C	78	ARG	2.1
1	C	79	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	62	GLY	2.0
1	A	161	ASN	2.0
1	B	135	VAL	2.0
1	A	604	VAL	2.0
1	D	174	VAL	2.0
1	D	87	GLU	2.0
1	D	247	SER	2.0
1	D	253	VAL	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
1	TRQ	B	697	16/17	0.96	0.06	14,20,27,30	0
1	TRQ	A	697	16/17	0.96	0.07	14,24,31,31	0
1	TRQ	D	697	16/17	0.97	0.06	15,24,33,40	0
1	TRQ	C	697	16/17	0.98	0.05	13,19,30,34	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
4	PEG	A	902	7/7	0.83	0.20	48,84,113,113	0
3	SO4	B	902	5/5	0.84	0.12	53,56,93,121	0
3	SO4	C	903	5/5	0.87	0.10	40,63,86,108	0
5	GLY	C	902	5/5	0.87	0.16	35,54,80,80	0
5	GLY	D	902	5/5	0.87	0.20	40,60,115,115	0
5	GLY	A	904	5/5	0.88	0.14	40,49,51,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GLY	A	903	5/5	0.94	0.13	31,52,90,90	0
2	MG	C	901	1/1	0.97	0.04	22,22,22,22	0
2	MG	D	901	1/1	0.98	0.03	28,28,28,28	0
2	MG	A	901	1/1	0.98	0.07	26,26,26,26	0
2	MG	B	901	1/1	0.99	0.04	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.