



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:37 pm BST

PDB ID : 6UBR
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

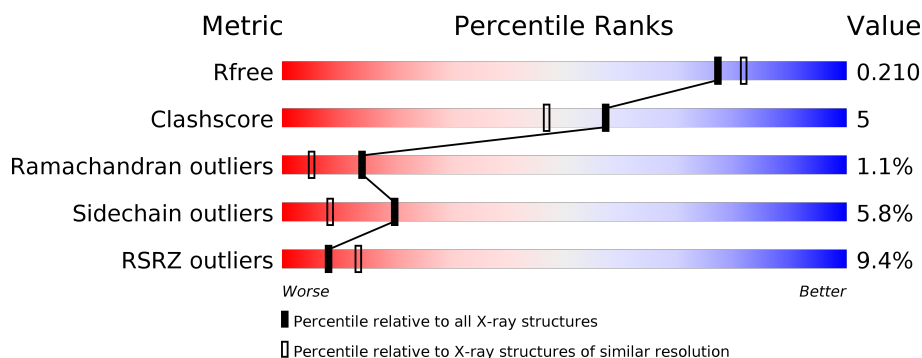
1 Overall quality at a glance

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on 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	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	816	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>• • •</div> </div> </div>
1	C	816	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>• 5%</div> </div> </div>
1	D	816	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div> </div>

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 crite-

ria:

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			

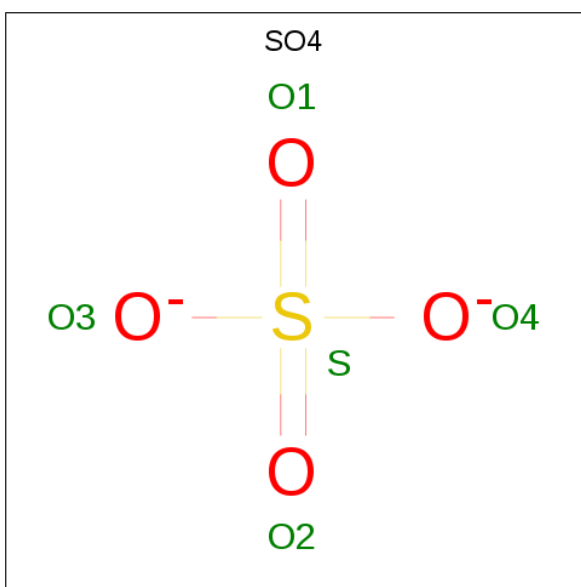
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

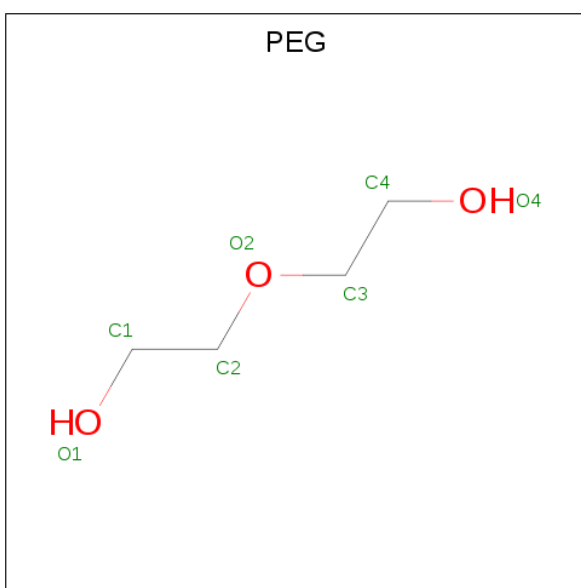
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



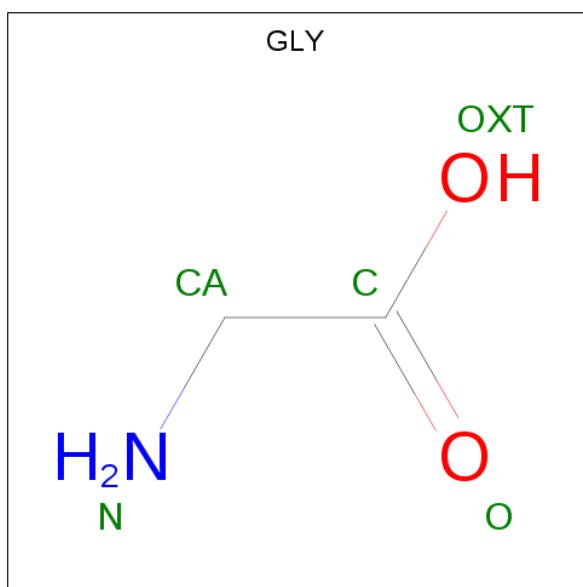
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



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		

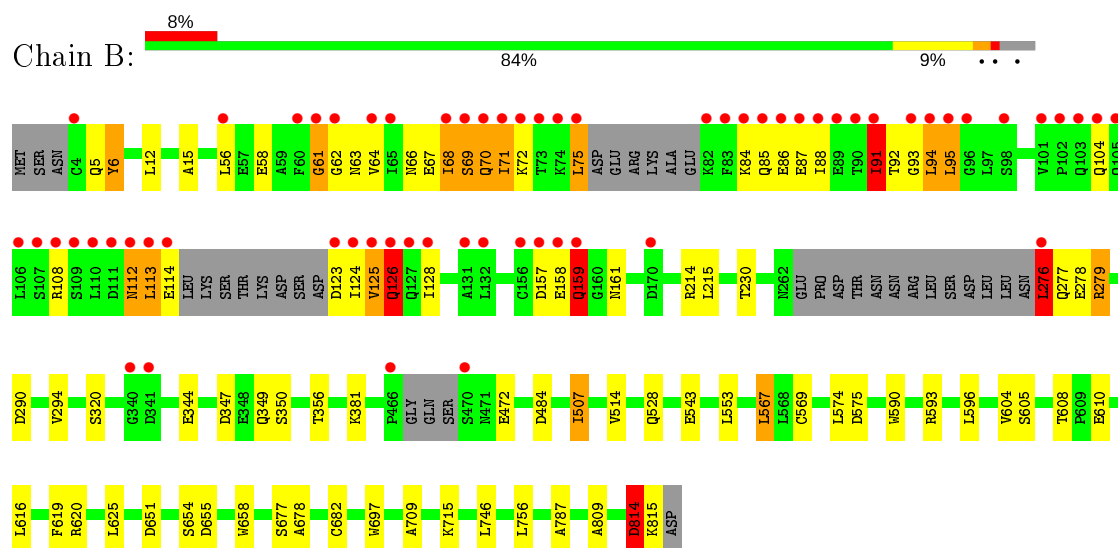
- Molecule 6 is water.

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		

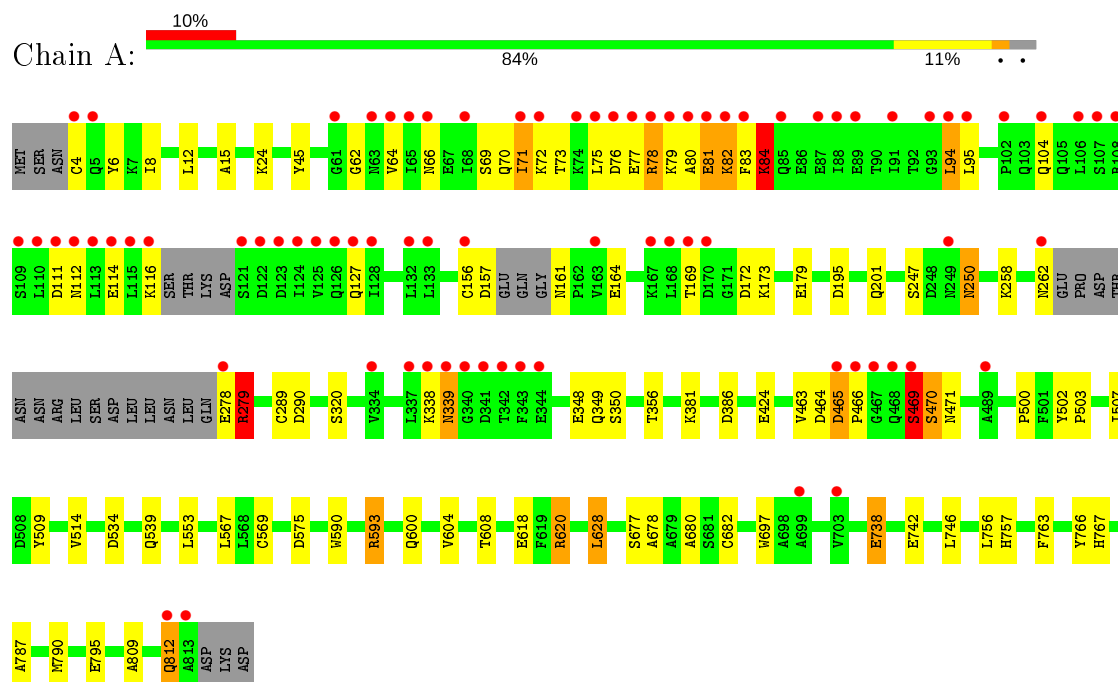
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

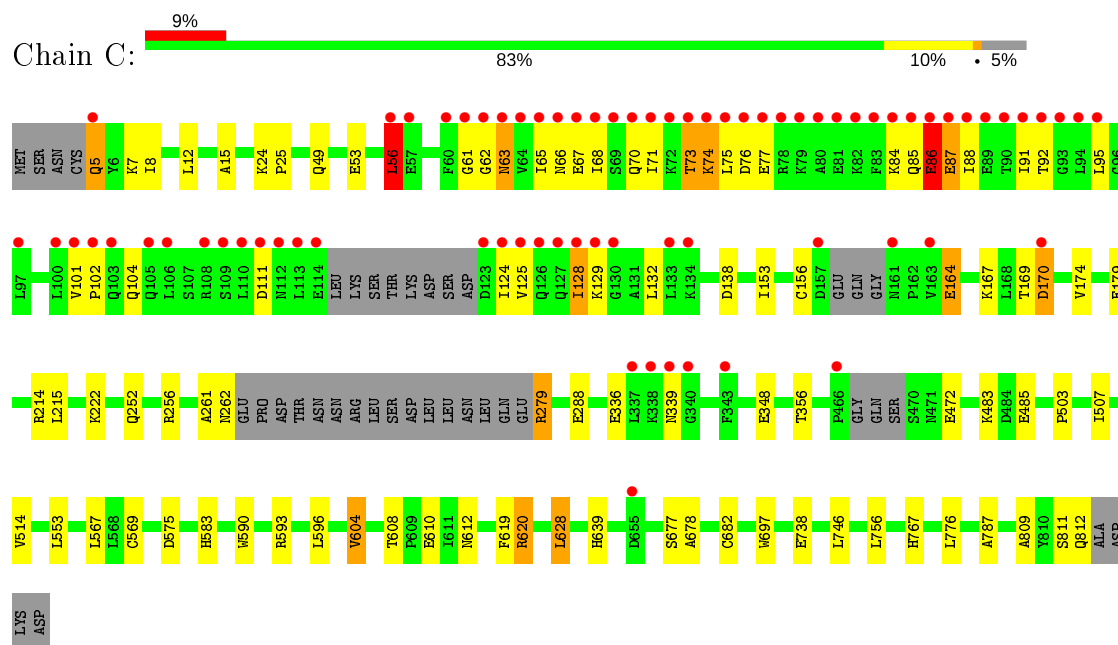
• Molecule 1: Uncharacterized protein



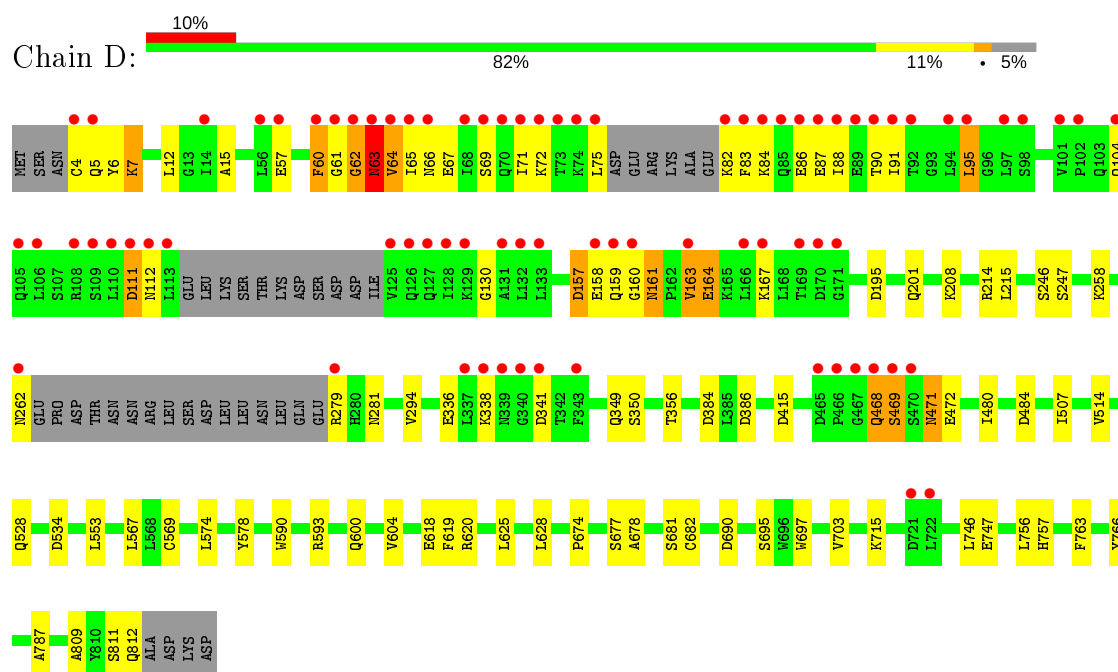
• Molecule 1: Uncharacterized protein



- 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 0.176 , 0.210	Depositor DCC
R_{free} test set	1998 reflections (0.74%)	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 , 50.3	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: TRQ, MG, PEG, SO4

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	0.29	0/6365	0.52	1/8662 (0.0%)
1	B	1.10	6/6328 (0.1%)	0.99	15/8614 (0.2%)
1	C	0.31	0/6296	0.53	1/8570 (0.0%)
1	D	0.28	0/6266	0.51	0/8530
All	All	0.60	6/25255 (0.0%)	0.67	17/34376 (0.0%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	TYR	CD1-CE1	51.20	2.16	1.39
1	B	6	TYR	CD2-CE2	50.66	2.15	1.39
1	B	6	TYR	CE1-CZ	-24.15	1.07	1.38
1	B	6	TYR	CE2-CZ	-23.80	1.07	1.38
1	B	6	TYR	CG-CD1	-17.45	1.16	1.39
1	B	6	TYR	CG-CD2	-17.27	1.16	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	TYR	CD1-CG-CD2	-33.84	80.68	117.90
1	B	6	TYR	CG-CD1-CE1	-29.33	97.83	121.30
1	B	6	TYR	CG-CD2-CE2	-29.21	97.94	121.30
1	B	6	TYR	CE1-CZ-CE2	-27.07	76.48	119.80
1	B	6	TYR	CB-CG-CD1	25.68	136.41	121.00
1	B	6	TYR	CB-CG-CD2	25.49	136.29	121.00
1	B	6	TYR	CZ-CE2-CD2	-21.24	100.69	119.80
1	B	6	TYR	CD1-CE1-CZ	-21.18	100.73	119.80
1	B	6	TYR	OH-CZ-CE2	8.12	142.02	120.10
1	B	6	TYR	CE1-CZ-OH	7.92	141.49	120.10
1	B	95	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	75	LEU	CB-CG-CD1	6.30	121.70	111.00
1	B	276	LEU	CB-CG-CD2	5.97	121.14	111.00
1	A	680	ALA	C-N-CA	5.89	136.43	121.70
1	C	56	LEU	CA-CB-CG	5.47	127.87	115.30
1	B	75	LEU	CB-CG-CD2	5.36	120.11	111.00
1	B	276	LEU	CB-CG-CD1	5.35	120.10	111.00

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

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	64	0
1	B	6197	5876	5973	52	0
1	C	6165	5873	5943	58	0
1	D	6134	5837	5912	64	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15	0
6	B	589	0	0	7	0
6	C	564	0	0	13	0
6	D	480	0	0	14	0
All	All	26935	23513	23853	236	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 (236) 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:D:811:SER:O	6:D:1002:HOH:O	1.99	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:814:ASP:CG	1:B:815:LYS:HA	2.08	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:277:GLN:OE1	6:B:1005:HOH:O	2.13	0.66
1:B:68:ILE:O	1:B:70:GLN:N	2.28	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
1:C:68:ILE:CG2	1:C:124:ILE:HD11	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CA	1:A:81:GLU:CB	2.73	0.62
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:A:682:CYS:SG	1:A:697:TRQ:HB3	2.43	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: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: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
1:A:618:GLU:OE2	1:A:620:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:D:63:ASN:OD1	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:A:795:GLU:OE2	6:A:1005:HOH:O	2.18	0.51
1:B:507:ILE:HD12	1:A:766:TYR:CD1	2.46	0.51
1:B:61:GLY:HA2	1:B:62:GLY:C	2.32	0.51
5:C:902:GLY:HA2	1:D:681[B]:SER:O	2.11	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: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:D:468:GLN:O	1:D:469:SER:HB3	2.13	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:C:261:ALA:O	1:C:262:ASN:HB2	2.13	0.48
1:D:111:ASP:CG	1:D:111:ASP:O	2.51	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:D:811:SER:O	1:D:812:GLN:HB2	2.13	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:160:GLY:CA	1:D:161:ASN:HB2	2.43	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:590:TRP:O	1:B:593:ARG:HG2	2.15	0.47
1:A:766:TYR:OH	5:A:904:GLY:O	2.25	0.47
1:B:787:ALA:HB1	1:B:809:ALA:HB1	1.96	0.47
1:D:677:SER:HB2	6:D:1249:HOH:O	2.15	0.47
1:A:503:PRO:HB3	1:A:507:ILE:HD12	1.97	0.47
1:A:250:ASN:HA	1:A:289:CYS:O	2.14	0.47
1:B:709:ALA:HB2	1:B:815:LYS:HG2	1.97	0.47
1:D:64:VAL:HG12	1:D:65:ILE:N	2.29	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:B:112:ASN:OD1	1:B:112:ASN:N	2.49	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: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:620:ARG:CZ	6:A:1006:HOH:O	2.56	0.46
1:A:76:ASP:O	1:A:78:ARG:N	2.49	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:D:95:LEU:HD23	1:D:95:LEU:O	2.16	0.45
1:A:79:LYS:HD3	1:A:79:LYS:HA	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: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
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:C:68:ILE:HG21	1:C:125:VAL:HG22	2.00	0.44
1:D:386:ASP:OD1	1:D:386:ASP:N	2.50	0.44
5:C:902:GLY:HA2	1:D:681[A]:SER:O	2.18	0.44
1:C:84:LYS:O	1:C:88:ILE:HG12	2.17	0.44
1:A:195:ASP:OD2	1:A:593:ARG:HD2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:514:VAL:HG12	2.19	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:B:514:VAL:O	1:B:514:VAL:HG12	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:C:124:ILE:HD12	1:C:124:ILE:C	2.39	0.42
1:A:386:ASP:OD1	1:A:386:ASP:N	2.52	0.42
1:D:590:TRP:O	1:D:593:ARG:CG	2.68	0.42
1:C:583:HIS:ND1	5:D:902:GLY:OXT	2.53	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:OE2	1:C:86:GLU:O	2.38	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
1:D:514:VAL:O	1:D:514:VAL:HG12	2.20	0.41
1:B:68:ILE:O	1:B:69:SER:C	2.58	0.41
1:B:84:LYS:HB2	1:B:87:GLU:HB2	2.02	0.41
1:C:619:PHE:O	1:C:620:ARG:HD2	2.20	0.41
1:C:70:GLN:O	1:C:74:LYS:HD3	2.20	0.41
1:D:349:GLN:O	1:D:620:ARG:HD2	2.19	0.41
1:A:464:ASP:O	1:A:465:ASP:C	2.58	0.41
1:B:68:ILE:C	1:B:70:GLN:N	2.74	0.41
1:B:157:ASP:HB2	1:B:161:ASN:H	1.86	0.41
1:D:262:ASN:HB2	1:D:279:ARG:HH12	1.86	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:D:88:ILE:HD11	1:D:111:ASP:HB2	2.02	0.41
1:C:583:HIS:O	5:D:902:GLY:HA2	2.20	0.41
1:B:655:ASP:O	1:B:658:TRP:HD1	2.03	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:A:738:GLU:O	1:A:742:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:ILE:HG21	1:D:507:ILE:HD11	2.02	0.41
1:C:169:THR:O	1:C:170:ASP:C	2.59	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: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 [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	780/816 (96%)	739 (95%)	32 (4%)	9 (1%)	13	4
1	B	773/816 (95%)	740 (96%)	24 (3%)	9 (1%)	13	4
1	C	768/816 (94%)	737 (96%)	24 (3%)	7 (1%)	17	8
1	D	768/816 (94%)	730 (95%)	28 (4%)	10 (1%)	12	3
All	All	3089/3264 (95%)	2946 (95%)	108 (4%)	35 (1%)	14	5

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

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Mol	Chain	Res	Type
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
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	684/710 (96%)	644 (94%)	40 (6%)	20	8
1	B	680/710 (96%)	634 (93%)	46 (7%)	16	5
1	C	676/710 (95%)	643 (95%)	33 (5%)	25	12
1	D	673/710 (95%)	635 (94%)	38 (6%)	21	9
All	All	2713/2840 (96%)	2556 (94%)	157 (6%)	20	8

All (157) 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
1	B	113	LEU
1	B	114	GLU
1	B	123	ASP
1	B	124	ILE
1	B	126	GLN
1	B	128	ILE
1	B	159	GLN
1	B	215	LEU
1	B	276	LEU
1	B	278	GLU
1	B	279	ARG
1	B	344	GLU
1	B	349	GLN
1	B	381	LYS

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Mol	Chain	Res	Type
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	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
1	A	82	LYS
1	A	84	LYS
1	A	95	LEU
1	A	104	GLN
1	A	111	ASP
1	A	114	GLU
1	A	116	LYS
1	A	127	GLN
1	A	164	GLU
1	A	173	LYS
1	A	247	SER
1	A	250	ASN
1	A	262	ASN
1	A	278	GLU
1	A	279	ARG
1	A	339	ASN
1	A	381	LYS
1	A	424	GLU

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Mol	Chain	Res	Type
1	A	465	ASP
1	A	534	ASP
1	A	553	LEU
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	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	85	GLN
1	C	86	GLU
1	C	91	ILE
1	C	95	LEU
1	C	104	GLN
1	C	128	ILE
1	C	153	ILE
1	C	164	GLU
1	C	167	LYS
1	C	174	VAL
1	C	215	LEU
1	C	279	ARG
1	C	336	GLU
1	C	553	LEU
1	C	569	CYS
1	C	575	ASP
1	C	596	LEU
1	C	604	VAL
1	C	608	THR
1	C	610	GLU
1	C	620	ARG
1	C	628	LEU

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Mol	Chain	Res	Type
1	C	677	SER
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	67	GLU
1	D	71	ILE
1	D	75	LEU
1	D	84	LYS
1	D	87	GLU
1	D	95	LEU
1	D	104	GLN
1	D	111	ASP
1	D	112	ASN
1	D	157	ASP
1	D	159	GLN
1	D	163	VAL
1	D	167	LYS
1	D	208	LYS
1	D	215	LEU
1	D	247	SER
1	D	294	VAL
1	D	336	GLU
1	D	338	LYS
1	D	341	ASP
1	D	468	GLN
1	D	471	ASN
1	D	534	ASP
1	D	553	LEU
1	D	569	CYS
1	D	574	LEU
1	D	578	TYR
1	D	625	LEU
1	D	628	LEU
1	D	715	LYS
1	D	746	LEU

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Mol	Chain	Res	Type
1	D	756	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	471	ASN
1	D	600	GLN

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	C	697	1	13,17,18	1.75	3 (23%)	14,24,26	1.68	3 (21%)
1	TRQ	A	697	1	13,17,18	1.76	2 (15%)	14,24,26	1.91	4 (28%)
1	TRQ	D	697	1	13,17,18	1.57	2 (15%)	14,24,26	1.86	4 (28%)
1	TRQ	B	697	1	13,17,18	1.61	2 (15%)	14,24,26	1.80	5 (35%)

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	C	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	A	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	D	697	1	-	0/4/19/21	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TRQ	B	697	1	-	0/4/19/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CE2-CZ2	-3.99	1.44	1.50
1	C	697	TRQ	CE2-CZ2	-3.86	1.45	1.50
1	B	697	TRQ	CE2-CZ2	-3.71	1.45	1.50
1	D	697	TRQ	CE2-CZ2	-3.40	1.45	1.50
1	A	697	TRQ	CB-CG	-3.00	1.47	1.51
1	C	697	TRQ	CB-CG	-2.94	1.47	1.51
1	B	697	TRQ	CB-CG	-2.65	1.48	1.51
1	D	697	TRQ	CB-CG	-2.39	1.48	1.51
1	C	697	TRQ	CD1-NE1	2.12	1.39	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	697	TRQ	CZ2-CE2-NE1	4.80	127.61	119.94
1	A	697	TRQ	CZ2-CE2-NE1	4.45	127.05	119.94
1	C	697	TRQ	CZ2-CE2-NE1	4.25	126.73	119.94
1	B	697	TRQ	CZ2-CE2-NE1	4.14	126.55	119.94
1	D	697	TRQ	CE3-CZ3-CH2	3.41	123.66	121.08
1	A	697	TRQ	CE3-CZ3-CH2	3.32	123.60	121.08
1	C	697	TRQ	O7-CZ2-CH2	2.69	122.16	119.00
1	B	697	TRQ	CE3-CZ3-CH2	2.67	123.10	121.08
1	C	697	TRQ	CE3-CZ3-CH2	2.61	123.06	121.08
1	B	697	TRQ	O7-CZ2-CH2	2.52	121.96	119.00
1	A	697	TRQ	O7-CZ2-CH2	2.48	121.91	119.00
1	D	697	TRQ	O7-CZ2-CE2	2.36	124.33	121.84
1	B	697	TRQ	CB-CG-CD1	-2.23	125.21	127.97
1	B	697	TRQ	O7-CZ2-CE2	2.19	124.15	121.84
1	D	697	TRQ	O7-CZ2-CH2	2.06	121.42	119.00
1	A	697	TRQ	CB-CG-CD1	-2.05	125.44	127.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
3	SO4	B	902	-	4,4,4	0.13	0	6,6,6	0.18	0
4	PEG	A	902	-	6,6,6	0.54	0	5,5,5	0.59	0
3	SO4	C	903	-	4,4,4	0.16	0	6,6,6	0.16	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
4	PEG	A	902	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) 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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	PEG	2	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	787/816 (96%)	0.38	79 (10%) 7 11	18, 33, 88, 136	0
1	B	781/816 (95%)	0.34	62 (7%) 12 19	17, 28, 94, 141	0
1	C	777/816 (95%)	0.47	74 (9%) 8 13	16, 29, 100, 161	0
1	D	775/816 (94%)	0.45	79 (10%) 6 11	20, 35, 99, 161	0
All	All	3120/3264 (95%)	0.41	294 (9%) 8 13	16, 31, 97, 161	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	68	ILE	14.1
1	C	65	ILE	12.5
1	C	83	PHE	12.1
1	C	88	ILE	11.5
1	C	79	LYS	11.0
1	C	62	GLY	10.4
1	C	94	LEU	10.2
1	B	125	VAL	10.1
1	C	66	ASN	9.9
1	B	110	LEU	9.6
1	C	75	LEU	9.5
1	D	75	LEU	9.3
1	B	83	PHE	9.0
1	C	113	LEU	8.7
1	D	73	THR	8.5
1	C	91	ILE	8.3
1	D	71	ILE	8.2
1	C	69	SER	8.0
1	D	83	PHE	8.0
1	C	110	LEU	8.0
1	A	116	LYS	7.9

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Mol	Chain	Res	Type	RSRZ
1	C	90	THR	7.9
1	C	125	VAL	7.8
1	C	95	LEU	7.8
1	B	73	THR	7.7
1	D	61	GLY	7.6
1	C	124	ILE	7.5
1	C	87	GLU	7.4
1	D	68	ILE	7.4
1	B	124	ILE	7.4
1	C	73	THR	7.3
1	D	468	GLN	7.3
1	C	80	ALA	7.3
1	B	68	ILE	7.2
1	C	114	GLU	7.2
1	C	61	GLY	7.2
1	B	71	ILE	7.1
1	A	468	GLN	7.0
1	A	115	LEU	7.0
1	D	86	GLU	7.0
1	C	71	ILE	6.9
1	C	112	ASN	6.8
1	C	81	GLU	6.8
1	C	64	VAL	6.7
1	A	83	PHE	6.7
1	A	813	ALA	6.7
1	D	94	LEU	6.6
1	D	158	GLU	6.5
1	D	65	ILE	6.5
1	D	126	GLN	6.4
1	B	61	GLY	6.4
1	C	70	GLN	6.4
1	B	72	LYS	6.3
1	B	65	ILE	6.3
1	B	123	ASP	6.2
1	B	113	LEU	6.2
1	B	82	LYS	6.1
1	D	88	ILE	6.1
1	D	104	GLN	6.1
1	B	158	GLU	6.1
1	D	91	ILE	6.1
1	C	77	GLU	6.1
1	D	82	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	127	GLN	6.0
1	C	60	PHE	6.0
1	B	127	GLN	5.9
1	C	109	SER	5.9
1	D	159	GLN	5.8
1	B	84	LYS	5.8
1	A	467	GLY	5.8
1	D	112	ASN	5.7
1	A	465	ASP	5.6
1	C	76	ASP	5.6
1	C	106	LEU	5.6
1	D	72	LYS	5.6
1	D	160	GLY	5.6
1	D	110	LEU	5.5
1	C	85	GLN	5.5
1	B	128	ILE	5.4
1	D	95	LEU	5.4
1	C	63	ASN	5.3
1	A	85	GLN	5.3
1	C	108	ARG	5.3
1	D	108	ARG	5.2
1	B	74	LYS	5.2
1	B	75	LEU	5.2
1	D	84	LYS	5.2
1	A	75	LEU	5.2
1	C	84	LYS	5.1
1	A	81	GLU	5.1
1	A	124	ILE	5.0
1	D	64	VAL	5.0
1	A	113	LEU	5.0
1	C	127	GLN	4.9
1	B	90	THR	4.9
1	D	69	SER	4.9
1	A	466	PRO	4.9
1	D	466	PRO	4.9
1	A	78	ARG	4.9
1	D	113	LEU	4.8
1	A	121	SER	4.7
1	D	66	ASN	4.7
1	B	112	ASN	4.7
1	B	91	ILE	4.6
1	D	467	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	62	GLY	4.5
1	A	112	ASN	4.5
1	C	126	GLN	4.5
1	D	87	GLU	4.4
1	B	470	SER	4.4
1	A	108	ARG	4.4
1	C	82	LYS	4.4
1	B	86	GLU	4.4
1	C	101	VAL	4.4
1	D	111	ASP	4.4
1	D	131	ALA	4.3
1	C	466	PRO	4.3
1	B	88	ILE	4.3
1	C	72	LYS	4.3
1	B	87	GLU	4.2
1	B	108	ARG	4.2
1	A	79	LYS	4.2
1	A	61	GLY	4.2
1	D	163	VAL	4.2
1	B	466	PRO	4.1
1	A	343	PHE	4.1
1	D	128	ILE	4.1
1	B	104	GLN	4.1
1	B	114	GLU	4.0
1	C	92	THR	4.0
1	B	89	GLU	4.0
1	A	127	GLN	4.0
1	A	82	LYS	4.0
1	B	106	LEU	3.9
1	A	122	ASP	3.9
1	C	133	LEU	3.9
1	C	123	ASP	3.9
1	B	111	ASP	3.8
1	B	4	CYS	3.8
1	D	469	SER	3.8
1	A	114	GLU	3.8
1	A	88	ILE	3.7
1	A	469	SER	3.7
1	D	56	LEU	3.7
1	B	85	GLN	3.7
1	D	85	GLN	3.7
1	C	170	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	130	GLY	3.7
1	A	163	VAL	3.7
1	D	129	LYS	3.6
1	D	4	CYS	3.6
1	A	77	GLU	3.6
1	C	97	LEU	3.5
1	C	74	LYS	3.5
1	A	128	ILE	3.4
1	A	95	LEU	3.4
1	A	110	LEU	3.4
1	D	90	THR	3.4
1	B	109	SER	3.4
1	B	276	LEU	3.4
1	A	125	VAL	3.4
1	D	337	LEU	3.4
1	C	78	ARG	3.3
1	A	64	VAL	3.3
1	D	465	ASP	3.3
1	A	111	ASP	3.3
1	B	131	ALA	3.3
1	B	64	VAL	3.3
1	A	76	ASP	3.3
1	B	93	GLY	3.2
1	C	89	GLU	3.2
1	D	74	LYS	3.2
1	A	63	ASN	3.2
1	A	71	ILE	3.2
1	B	62	GLY	3.2
1	A	4	CYS	3.2
1	A	156	CYS	3.2
1	B	103	GLN	3.2
1	C	56	LEU	3.1
1	A	167	LYS	3.1
1	B	102	PRO	3.1
1	D	60	PHE	3.1
1	A	91	ILE	3.1
1	C	129	LYS	3.1
1	A	262	ASN	3.1
1	A	170	ASP	3.1
1	A	102	PRO	3.1
1	B	107	SER	3.1
1	D	721	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	65	ILE	3.1
1	A	169	THR	3.0
1	A	340	GLY	3.0
1	D	106	LEU	3.0
1	C	163	VAL	3.0
1	B	126	GLN	2.9
1	D	89	GLU	2.9
1	D	340	GLY	2.9
1	B	70	GLN	2.9
1	B	94	LEU	2.9
1	C	339	ASN	2.9
1	C	161	ASN	2.9
1	D	132	LEU	2.8
1	C	103	GLN	2.8
1	A	337	LEU	2.8
1	A	123	ASP	2.8
1	D	63	ASN	2.8
1	A	72	LYS	2.8
1	A	74	LYS	2.8
1	D	57	GLU	2.8
1	D	125	VAL	2.8
1	A	489	ALA	2.7
1	D	169	THR	2.7
1	A	5	GLN	2.7
1	D	171	GLY	2.7
1	B	159	GLN	2.7
1	D	109	SER	2.7
1	D	97	LEU	2.7
1	D	338	LYS	2.7
1	D	102	PRO	2.7
1	D	339	ASN	2.7
1	B	60	PHE	2.7
1	C	86	GLU	2.7
1	B	95	LEU	2.6
1	D	279	ARG	2.6
1	C	111	ASP	2.6
1	D	98	SER	2.6
1	C	343	PHE	2.6
1	A	168	LEU	2.6
1	A	126	GLN	2.6
1	D	341	ASP	2.5
1	C	93	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	132	LEU	2.5
1	C	337	LEU	2.5
1	D	133	LEU	2.5
1	A	278	GLU	2.5
1	A	344	GLU	2.5
1	A	106	LEU	2.5
1	A	338	LYS	2.5
1	B	156	CYS	2.5
1	C	5	GLN	2.4
1	A	107	SER	2.4
1	A	109	SER	2.4
1	D	92	THR	2.4
1	D	70	GLN	2.4
1	B	101	VAL	2.4
1	A	68	ILE	2.4
1	A	334	VAL	2.4
1	B	341	ASP	2.4
1	A	66	ASN	2.4
1	C	128	ILE	2.4
1	C	100	LEU	2.3
1	A	89	GLU	2.3
1	A	132	LEU	2.3
1	D	14	ILE	2.3
1	A	699	ALA	2.3
1	A	703	VAL	2.3
1	A	104	GLN	2.3
1	D	105	GLN	2.3
1	B	98	SER	2.3
1	D	470	SER	2.3
1	A	339	ASN	2.2
1	D	262	ASN	2.2
1	A	341	ASP	2.2
1	D	166	LEU	2.2
1	D	722	LEU	2.2
1	B	105	GLN	2.2
1	C	67	GLU	2.2
1	C	134	LYS	2.2
1	C	338	LYS	2.2
1	C	157	ASP	2.2
1	D	170	ASP	2.2
1	C	105	GLN	2.2
1	A	133	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	170	ASP	2.2
1	B	69	SER	2.2
1	A	80	ALA	2.2
1	A	87	GLU	2.1
1	A	94	LEU	2.1
1	A	93	GLY	2.1
1	B	96	GLY	2.1
1	D	343	PHE	2.1
1	A	342	THR	2.1
1	D	5	GLN	2.1
1	C	340	GLY	2.1
1	C	57	GLU	2.1
1	D	167	LYS	2.1
1	D	101	VAL	2.1
1	A	812	GLN	2.1
1	B	340	GLY	2.1
1	B	157	ASP	2.0
1	C	102	PRO	2.0
1	B	56	LEU	2.0
1	C	655	ASP	2.0
1	A	249	ASN	2.0

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

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	A	697	16/17	0.95	0.18	14,24,31,31	0
1	TRQ	D	697	16/17	0.96	0.16	15,24,33,40	0
1	TRQ	B	697	16/17	0.96	0.18	14,20,27,30	0
1	TRQ	C	697	16/17	0.98	0.14	13,19,30,34	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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	0.65	0.25	48,84,113,113	0
5	GLY	D	902	5/5	0.82	0.24	40,60,115,115	0
5	GLY	C	902	5/5	0.82	0.21	35,54,80,80	0
5	GLY	A	904	5/5	0.86	0.21	40,49,51,64	0
3	SO4	B	902	5/5	0.93	0.20	53,56,93,121	0
3	SO4	C	903	5/5	0.94	0.15	40,63,86,108	0
5	GLY	A	903	5/5	0.95	0.16	31,52,90,90	0
2	MG	D	901	1/1	0.98	0.18	28,28,28,28	0
2	MG	C	901	1/1	0.99	0.11	22,22,22,22	0
2	MG	A	901	1/1	0.99	0.07	26,26,26,26	0
2	MG	B	901	1/1	0.99	0.07	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.