



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2017 – 02:19 AM EDT

PDB ID : 4K5Y
Title : Crystal structure of human corticotropin-releasing factor receptor 1 (CRF1R) in complex with the antagonist CP-376395
Authors : Hollenstein, K.; Kean, J.; Bortolato, A.; Cheng, R.K.Y.; Dore, A.S.; Jazayeri, A.; Cooke, R.M.; Weir, M.; Marshall, F.H.
Deposited on : unknown
Resolution : 2.98 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

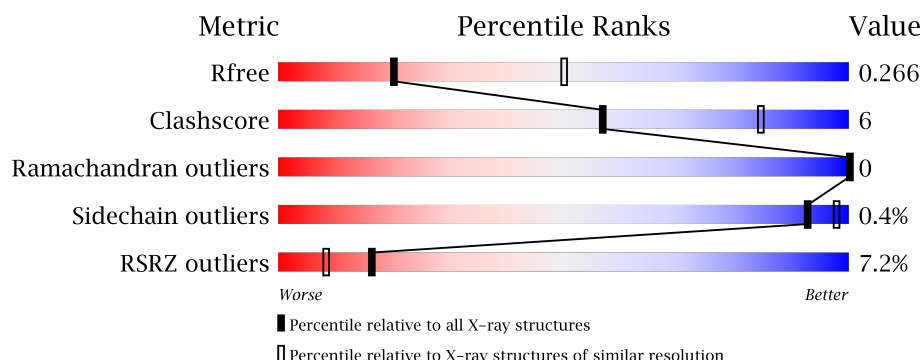
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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. 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	441	<div> <div>7%</div> <div>79% 13% 8%</div> </div>
1	B	441	<div> <div>4%</div> <div>78% 12% 10%</div> </div>
1	C	441	<div> <div>6%</div> <div>50% 6% 44%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLC	A	503	-	-	-	X
5	SO4	A	504	-	-	X	-
6	PGW	B	502	-	-	-	X
6	PGW	B	504	-	-	-	X
7	1PE	B	505	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8823 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 Corticotropin-releasing factor receptor 1, T4-Lysozyme chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3278	2145	562	554	17			
1	B	396	Total	C	N	O	S	0	0	0
			3194	2091	547	539	17			
1	C	248	Total	C	N	O	S	0	0	0
			2005	1341	330	321	13			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	INITIATING METHIONINE	UNP P34998
A	120	ALA	VAL	ENGINEERED MUTATION	UNP P34998
A	144	ALA	LEU	ENGINEERED MUTATION	UNP P34998
A	156	ALA	TRP	ENGINEERED MUTATION	UNP P34998
A	160	ALA	SER	ENGINEERED MUTATION	UNP P34998
A	1040	SER	ASN	ENGINEERED MUTATION	UNP P00720
A	1041	VAL	ALA	ENGINEERED MUTATION	UNP P00720
A	1054	SER	CYS	ENGINEERED MUTATION	UNP P00720
A	1097	SER	CYS	ENGINEERED MUTATION	UNP P00720
A	1151	ALA	THR	ENGINEERED MUTATION	UNP P00720
A	228	ALA	LYS	ENGINEERED MUTATION	UNP P34998
A	260	ALA	PHE	ENGINEERED MUTATION	UNP P34998
A	277	ALA	ILE	ENGINEERED MUTATION	UNP P34998
A	309	ALA	TYR	ENGINEERED MUTATION	UNP P34998
A	330	ALA	PHE	ENGINEERED MUTATION	UNP P34998
A	349	ALA	SER	ENGINEERED MUTATION	UNP P34998
A	363	ALA	TYR	ENGINEERED MUTATION	UNP P34998
A	374	ALA	-	EXPRESSION TAG	UNP P34998
A	375	ALA	-	EXPRESSION TAG	UNP P34998
A	376	ALA	-	EXPRESSION TAG	UNP P34998
A	377	HIS	-	EXPRESSION TAG	UNP P34998
A	378	HIS	-	EXPRESSION TAG	UNP P34998

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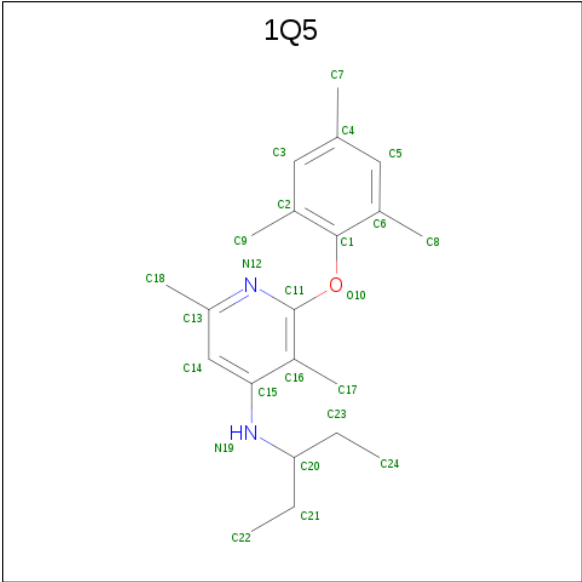
Chain	Residue	Modelled	Actual	Comment	Reference
A	379	HIS	-	EXPRESSION TAG	UNP P34998
A	380	HIS	-	EXPRESSION TAG	UNP P34998
A	381	HIS	-	EXPRESSION TAG	UNP P34998
A	382	HIS	-	EXPRESSION TAG	UNP P34998
A	383	HIS	-	EXPRESSION TAG	UNP P34998
A	384	HIS	-	EXPRESSION TAG	UNP P34998
A	385	HIS	-	EXPRESSION TAG	UNP P34998
A	386	HIS	-	EXPRESSION TAG	UNP P34998
B	103	MET	-	INITIATING METHIONINE	UNP P34998
B	120	ALA	VAL	ENGINEERED MUTATION	UNP P34998
B	144	ALA	LEU	ENGINEERED MUTATION	UNP P34998
B	156	ALA	TRP	ENGINEERED MUTATION	UNP P34998
B	160	ALA	SER	ENGINEERED MUTATION	UNP P34998
B	1040	SER	ASN	ENGINEERED MUTATION	UNP P00720
B	1041	VAL	ALA	ENGINEERED MUTATION	UNP P00720
B	1054	SER	CYS	ENGINEERED MUTATION	UNP P00720
B	1097	SER	CYS	ENGINEERED MUTATION	UNP P00720
B	1151	ALA	THR	ENGINEERED MUTATION	UNP P00720
B	228	ALA	LYS	ENGINEERED MUTATION	UNP P34998
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B	309	ALA	TYR	ENGINEERED MUTATION	UNP P34998
B	330	ALA	PHE	ENGINEERED MUTATION	UNP P34998
B	349	ALA	SER	ENGINEERED MUTATION	UNP P34998
B	363	ALA	TYR	ENGINEERED MUTATION	UNP P34998
B	374	ALA	-	EXPRESSION TAG	UNP P34998
B	375	ALA	-	EXPRESSION TAG	UNP P34998
B	376	ALA	-	EXPRESSION TAG	UNP P34998
B	377	HIS	-	EXPRESSION TAG	UNP P34998
B	388	HIS	-	EXPRESSION TAG	UNP P34998
B	389	HIS	-	EXPRESSION TAG	UNP P34998
B	390	HIS	-	EXPRESSION TAG	UNP P34998
B	391	HIS	-	EXPRESSION TAG	UNP P34998
B	392	HIS	-	EXPRESSION TAG	UNP P34998
B	393	HIS	-	EXPRESSION TAG	UNP P34998
B	394	HIS	-	EXPRESSION TAG	UNP P34998
B	395	HIS	-	EXPRESSION TAG	UNP P34998
B	396	HIS	-	EXPRESSION TAG	UNP P34998
C	103	MET	-	INITIATING METHIONINE	UNP P34998
C	120	ALA	VAL	ENGINEERED MUTATION	UNP P34998
C	144	ALA	LEU	ENGINEERED MUTATION	UNP P34998
C	156	ALA	TRP	ENGINEERED MUTATION	UNP P34998

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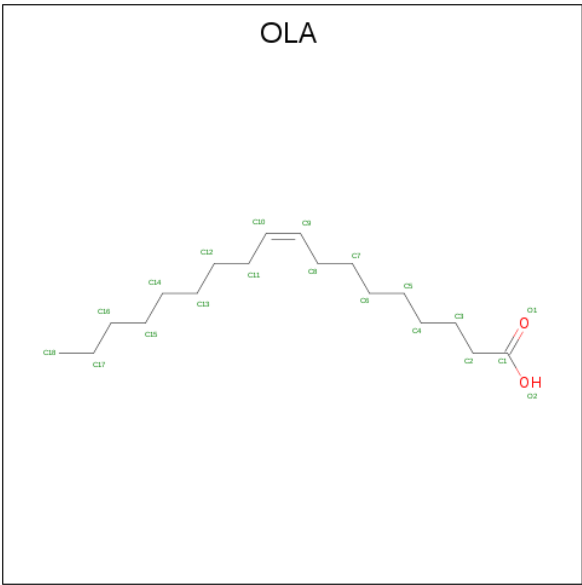
Chain	Residue	Modelled	Actual	Comment	Reference
C	160	ALA	SER	ENGINEERED MUTATION	UNP P34998
C	1040	SER	ASN	ENGINEERED MUTATION	UNP P00720
C	1041	VAL	ALA	ENGINEERED MUTATION	UNP P00720
C	1054	SER	CYS	ENGINEERED MUTATION	UNP P00720
C	1097	SER	CYS	ENGINEERED MUTATION	UNP P00720
C	1151	ALA	THR	ENGINEERED MUTATION	UNP P00720
C	228	ALA	LYS	ENGINEERED MUTATION	UNP P34998
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C	277	ALA	ILE	ENGINEERED MUTATION	UNP P34998
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C	330	ALA	PHE	ENGINEERED MUTATION	UNP P34998
C	349	ALA	SER	ENGINEERED MUTATION	UNP P34998
C	363	ALA	TYR	ENGINEERED MUTATION	UNP P34998
C	374	ALA	-	EXPRESSION TAG	UNP P34998
C	375	ALA	-	EXPRESSION TAG	UNP P34998
C	376	ALA	-	EXPRESSION TAG	UNP P34998
C	377	HIS	-	EXPRESSION TAG	UNP P34998
C	378	HIS	-	EXPRESSION TAG	UNP P34998
C	379	HIS	-	EXPRESSION TAG	UNP P34998
C	380	HIS	-	EXPRESSION TAG	UNP P34998
C	381	HIS	-	EXPRESSION TAG	UNP P34998
C	382	HIS	-	EXPRESSION TAG	UNP P34998
C	383	HIS	-	EXPRESSION TAG	UNP P34998
C	384	HIS	-	EXPRESSION TAG	UNP P34998
C	385	HIS	-	EXPRESSION TAG	UNP P34998
C	386	HIS	-	EXPRESSION TAG	UNP P34998

- Molecule 2 is 3,6-dimethyl-N-(pentan-3-yl)-2-(2,4,6-trimethylphenoxy)pyridin-4-amine (three-letter code: 1Q5) (formula: C₂₁H₃₀N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	21	2	1		
2	B	1	Total	C	N	O	0	0
			24	21	2	1		
2	C	1	Total	C	N	O	0	0
			24	21	2	1		

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



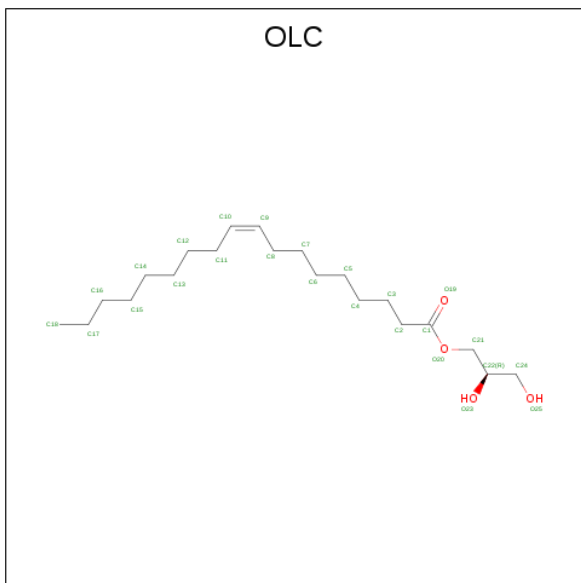
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			13	13		

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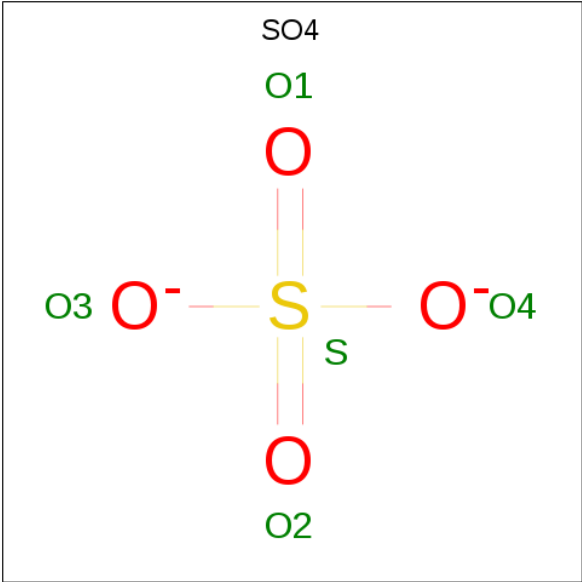
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



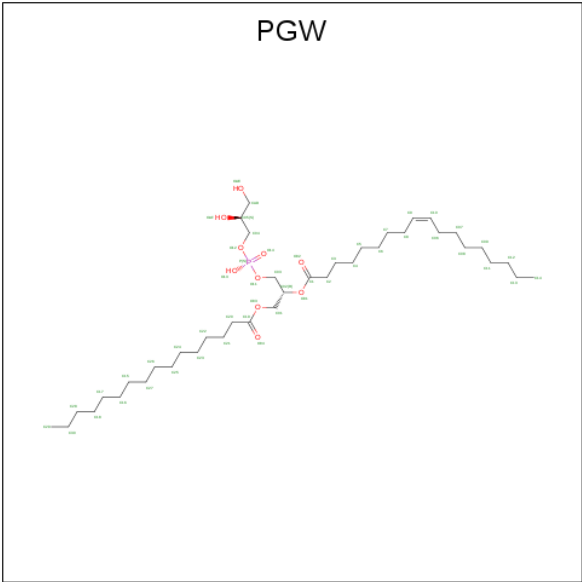
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



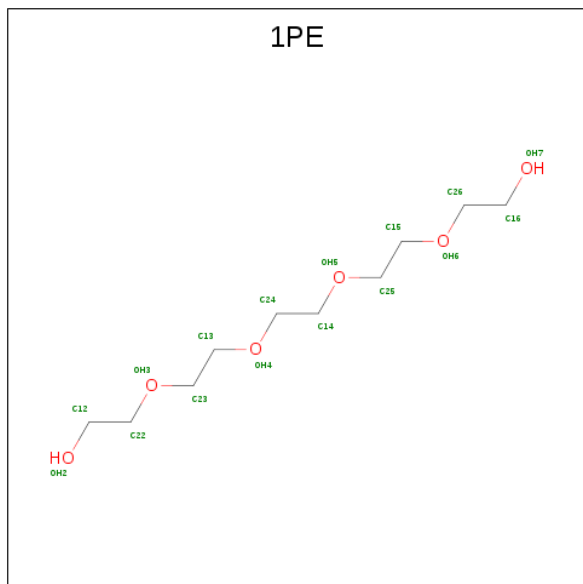
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			39	30	8	1		
6	B	1	Total	C	O	P	0	0
			46	37	8	1		
6	B	1	Total	C	O		0	0
			37	32	5			

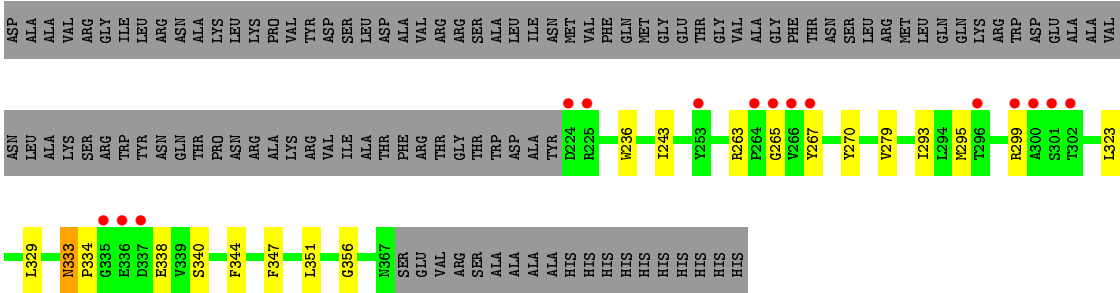
- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	O	0	0
			4	4		
8	B	4	Total	O	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.56Å 123.97Å 166.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.14 – 2.98 34.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	85.7 (34.14-2.98) 85.7 (34.15-2.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.242 , 0.265 0.239 , 0.266	Depositor DCC
R_{free} test set	1586 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8823	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLC, 1PE, 1Q5, PGW, 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	0.62	0/3358	0.68	3/4556 (0.1%)
1	B	0.65	0/3271	0.65	1/4435 (0.0%)
1	C	0.60	0/2063	0.69	0/2810
All	All	0.63	0/8692	0.67	4/11801 (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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LYS	N-CA-C	-7.98	89.46	111.00
1	B	296	THR	N-CA-C	6.72	129.15	111.00
1	A	1048	LYS	CD-CE-NZ	-6.53	96.68	111.70
1	A	1007	LEU	CB-CG-CD2	-5.55	101.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	GLU	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3278	0	3333	40	1
1	B	3194	0	3247	40	1
1	C	2005	0	2038	19	1
2	A	24	0	30	2	0
2	B	24	0	30	5	0
2	C	24	0	30	3	0
3	A	13	0	23	1	0
3	C	20	0	33	1	0
4	A	50	0	80	4	0
4	B	25	0	40	2	0
5	A	5	0	0	1	1
5	B	15	0	0	0	1
6	B	122	0	174	10	0
7	B	16	0	22	0	0
8	A	4	0	0	0	0
8	B	4	0	0	1	0
All	All	8823	0	9080	102	3

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 6.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLU:HB2	1:C:340:SER:H	1.44	0.82
1:B:329:LEU:HB3	1:B:344:PHE:HE1	1.48	0.77
1:A:1006:MET:HG2	1:A:1007:LEU:HD12	1.69	0.75
1:A:263:ARG:O	1:A:265:GLY:HA3	1.87	0.74
1:C:263:ARG:O	1:C:265:GLY:HA3	1.92	0.70
1:A:367:ASN:ND2	4:A:502:OLC:O25	2.28	0.67
1:B:1024:TYR:HB3	1:B:1032:LEU:HD11	1.77	0.66
1:B:232:ILE:HD11	6:B:502:PGW:H01A	1.77	0.66
1:A:197:TYR:HA	1:A:243:ILE:HG13	1.78	0.65
1:A:357:PHE:HE1	4:A:502:OLC:H11A	1.63	0.63
1:B:1087:VAL:HG21	1:B:1118:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1025:TYR:O	1:B:1032:LEU:HD12	2.00	0.61
1:A:126:GLY:HA3	1:A:353:SER:HB2	1.82	0.61
1:B:320:LEU:HD22	2:B:401:1Q5:H14	1.84	0.60
1:A:140:LEU:HD13	4:A:502:OLC:H22	1.85	0.58
1:A:1041:VAL:O	1:A:1045:GLU:HG2	2.04	0.58
1:B:323:LEU:HD22	1:B:355:GLN:HG2	1.86	0.58
1:A:347:PHE:CE2	1:A:351:LEU:HD11	2.39	0.57
1:C:218:VAL:HG22	1:C:293:ILE:HD12	1.86	0.55
1:B:203:PHE:CE1	2:B:401:1Q5:H24	2.42	0.55
1:C:334:PRO:HD3	1:C:344:PHE:CZ	2.42	0.55
1:A:203:PHE:CE1	2:A:401:1Q5:H24	2.42	0.54
1:B:199:HIS:HE1	6:B:504:PGW:H02	1.72	0.54
1:B:250:LYS:O	1:B:254:ASP:O	2.26	0.53
1:B:320:LEU:HB3	1:B:321:PRO:HD3	1.90	0.53
1:A:248:ILE:HD12	4:B:501:OLC:H8A	1.92	0.52
1:A:248:ILE:HG23	1:B:230:MET:HE1	1.93	0.51
1:B:135:LEU:HD22	6:B:502:PGW:H11A	1.93	0.51
6:B:504:PGW:H2	6:B:504:PGW:H24	1.93	0.50
1:A:1014:ARG:HH11	1:B:256:GLU:CG	2.24	0.49
1:C:197:TYR:HB2	1:C:243:ILE:HG13	1.94	0.49
1:C:323:LEU:HD12	2:C:401:1Q5:H7	1.93	0.49
1:A:256:GLU:OE2	1:A:263:ARG:HG3	2.12	0.49
1:A:217:ILE:HD12	1:A:290:ILE:HG23	1.95	0.48
1:C:203:PHE:CE1	2:C:401:1Q5:H24	2.48	0.48
1:B:283:ASN:ND2	2:B:401:1Q5:H1	2.29	0.48
1:B:280:LEU:HD23	6:B:504:PGW:H06A	1.95	0.48
1:A:1006:MET:HE1	1:A:1097:SER:HB3	1.95	0.48
1:A:1014:ARG:NH1	1:B:254:ASP:OD1	2.47	0.48
1:C:267:TYR:HB3	1:C:270:TYR:CD1	2.49	0.48
1:A:1118:LEU:HD23	1:A:1121:LEU:HD12	1.94	0.48
1:A:1007:LEU:CD2	1:A:1104:PHE:HD2	2.27	0.48
1:C:207:PHE:HB2	1:C:279:VAL:CG1	2.43	0.48
1:A:1087:VAL:HG21	1:A:1118:LEU:HB3	1.96	0.47
1:B:234:ILE:HD11	4:B:501:OLC:H4A	1.95	0.47
1:B:329:LEU:HB3	1:B:344:PHE:CE1	2.38	0.47
1:A:1078:ILE:HD11	1:A:1103:VAL:HG21	1.97	0.47
1:A:1073:ALA:HA	1:A:1076:ARG:HE	1.79	0.47
1:A:207:PHE:HB2	1:A:279:VAL:CG1	2.45	0.47
1:B:283:ASN:HD22	2:B:401:1Q5:H1	1.80	0.47
1:B:204:PHE:O	1:B:207:PHE:HB3	2.15	0.47
1:C:334:PRO:HD3	1:C:344:PHE:CE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:O	1:B:200:VAL:HG23	2.16	0.46
1:B:326:THR:HG21	1:B:352:GLU:HG3	1.98	0.46
1:A:1117:SER:N	5:A:504:SO4:O3	2.44	0.46
4:A:503:OLC:H3	1:B:189:ARG:NH2	2.31	0.46
1:C:333:ASN:HD22	1:C:333:ASN:C	2.16	0.46
1:C:201:THR:HG21	1:C:236:TRP:CZ3	2.51	0.45
1:A:321:PRO:O	1:A:325:ILE:HG22	2.17	0.45
1:C:210:GLY:HA2	2:C:401:1Q5:H9	1.97	0.45
3:C:501:OLA:H112	3:C:501:OLA:H82	1.75	0.45
6:B:502:PGW:H6	6:B:502:PGW:H22A	1.99	0.45
1:A:1006:MET:HG3	1:A:1161:TYR:CZ	2.52	0.45
1:A:256:GLU:CD	1:A:263:ARG:HE	2.19	0.45
1:B:207:PHE:HB2	1:B:279:VAL:CG1	2.47	0.45
1:A:183:SER:OG	1:A:185:VAL:HG23	2.17	0.44
1:B:284:PHE:CE1	1:B:320:LEU:HD21	2.53	0.44
1:B:205:TRP:CE2	1:B:235:GLY:HA3	2.53	0.44
1:A:1025:TYR:O	1:A:1032:LEU:HD12	2.18	0.44
1:A:293:ILE:HA	1:A:296:THR:OG1	2.18	0.44
1:A:1117:SER:O	1:A:1121:LEU:HG	2.18	0.44
1:A:325:ILE:HG23	1:A:351:LEU:HD13	1.99	0.44
1:A:1159:ASP:O	1:A:225:ARG:HG3	2.17	0.43
1:A:1077:GLY:HA3	1:A:1108:GLU:OE2	2.18	0.43
1:A:329:LEU:HD22	1:A:344:PHE:HE1	1.84	0.43
1:C:130:SER:HB3	1:C:356:GLY:HA3	2.00	0.43
1:A:325:ILE:HD13	1:A:347:PHE:HE2	1.82	0.43
3:A:501:OLA:H112	3:A:501:OLA:H82	1.84	0.42
1:B:270:TYR:CD2	6:B:504:PGW:H17	2.54	0.42
1:B:129:ILE:HA	6:B:503:PGW:H18A	2.01	0.42
1:B:138:PHE:CE2	6:B:502:PGW:H08	2.55	0.42
1:B:284:PHE:CZ	1:B:320:LEU:HD21	2.55	0.42
2:B:401:1Q5:H8	2:B:401:1Q5:H4	1.78	0.42
1:B:1101:ASN:OD1	8:B:602:HOH:O	2.22	0.42
1:B:199:HIS:CE1	6:B:504:PGW:H02	2.54	0.42
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.89	0.42
1:A:295:MET:O	1:A:299:ARG:HG3	2.20	0.42
1:B:238:VAL:O	1:B:241:PRO:HD2	2.20	0.42
1:A:1046:LEU:HD21	1:A:1058:ILE:HG23	2.01	0.41
1:C:151:ARG:HG2	1:C:155:HIS:CE1	2.55	0.41
1:C:329:LEU:HD22	1:C:344:PHE:CE2	2.55	0.41
1:A:130:SER:HB3	1:A:356:GLY:HA3	2.02	0.41
1:B:298:LEU:HD13	1:B:306:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1078:ILE:HD11	1:B:1103:VAL:HG21	2.03	0.41
2:A:401:1Q5:H4	2:A:401:1Q5:H8	1.77	0.41
1:C:295:MET:O	1:C:299:ARG:HB2	2.21	0.41
1:B:1125:ARG:HH11	1:B:1128:GLU:CD	2.24	0.40
1:C:207:PHE:HB2	1:C:279:VAL:HG13	2.03	0.40
1:C:347:PHE:CZ	1:C:351:LEU:HD11	2.56	0.40
1:B:240:PHE:HB3	1:B:241:PRO:HD3	2.03	0.40
1:B:233:CYS:O	1:B:238:VAL:HG23	2.21	0.40
1:B:181:HIS:NE2	1:B:257:LYS:HB3	2.36	0.40

All (3) 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:A:1137:ARG:NH1	5:B:506:SO4:O1[1_655]	2.16	0.04
1:B:1137:ARG:NH1	5:A:504:SO4:O2[1_455]	2.17	0.03
1:C:270:TYR:OH	1:C:338:GLU:OE1[2_556]	2.19	0.01

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	403/441 (91%)	394 (98%)	9 (2%)	0	100	100
1	B	390/441 (88%)	383 (98%)	7 (2%)	0	100	100
1	C	244/441 (55%)	240 (98%)	4 (2%)	0	100	100
All	All	1037/1323 (78%)	1017 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/374 (92%)	344 (100%)	1 (0%)	94	98
1	B	335/374 (90%)	333 (99%)	2 (1%)	89	96
1	C	211/374 (56%)	210 (100%)	1 (0%)	91	97
All	All	891/1122 (79%)	887 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	TYR
1	B	283	ASN
1	B	354	PHE
1	C	333	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	367	ASN
1	C	333	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 carbohydrates in this entry.

5.6 Ligand geometry

16 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	1Q5	A	401	-	24,25,25	1.57	3 (12%)	28,35,35	1.96	8 (28%)
3	OLA	A	501	-	12,12,19	0.30	0	11,11,19	0.68	0
4	OLC	A	502	-	24,24,24	0.80	2 (8%)	25,25,25	1.02	1 (4%)
4	OLC	A	503	-	24,24,24	0.83	2 (8%)	25,25,25	1.02	2 (8%)
5	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.10	0
2	1Q5	B	401	-	24,25,25	1.55	3 (12%)	28,35,35	1.87	7 (25%)
4	OLC	B	501	-	24,24,24	0.79	2 (8%)	25,25,25	1.01	1 (4%)
6	PGW	B	502	-	38,38,50	0.95	3 (7%)	42,43,56	1.28	3 (7%)
6	PGW	B	503	-	45,45,50	0.87	3 (6%)	49,50,56	1.20	2 (4%)
6	PGW	B	504	-	36,36,50	0.91	3 (8%)	38,38,56	1.27	2 (5%)
7	1PE	B	505	-	15,15,15	0.52	0	14,14,14	0.86	0
5	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	507	-	4,4,4	0.14	0	6,6,6	0.13	0
5	SO4	B	508	-	4,4,4	0.18	0	6,6,6	0.07	0
2	1Q5	C	401	-	24,25,25	1.54	3 (12%)	28,35,35	1.82	6 (21%)
3	OLA	C	501	-	16,19,19	0.28	0	15,19,19	0.84	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
2	1Q5	A	401	-	-	0/12/12/12	0/2/2/2
3	OLA	A	501	-	-	0/10/10/17	0/0/0/0
4	OLC	A	502	-	-	0/24/24/24	0/0/0/0
4	OLC	A	503	-	-	0/24/24/24	0/0/0/0
5	SO4	A	504	-	-	0/0/0/0	0/0/0/0
2	1Q5	B	401	-	-	0/12/12/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	B	501	-	-	0/24/24/24	0/0/0/0
6	PGW	B	502	-	-	0/40/40/55	0/0/0/0
6	PGW	B	503	-	-	0/47/47/55	0/0/0/0
6	PGW	B	504	-	-	0/38/38/55	0/0/0/0
7	1PE	B	505	-	-	0/13/13/13	0/0/0/0
5	SO4	B	506	-	-	0/0/0/0	0/0/0/0
5	SO4	B	507	-	-	0/0/0/0	0/0/0/0
5	SO4	B	508	-	-	0/0/0/0	0/0/0/0
2	1Q5	C	401	-	-	0/12/12/12	0/2/2/2
3	OLA	C	501	-	-	0/15/17/17	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	503	PGW	O01-C1	-3.04	1.25	1.34
6	B	504	PGW	O01-C1	-2.98	1.25	1.34
6	B	502	PGW	O01-C1	-2.84	1.26	1.34
6	B	503	PGW	O03-C19	-2.60	1.25	1.33
4	B	501	OLC	O20-C1	-2.58	1.25	1.33
4	A	502	OLC	O20-C1	-2.49	1.25	1.33
6	B	504	PGW	O03-C19	-2.46	1.26	1.33
6	B	502	PGW	O03-C19	-2.43	1.26	1.33
4	A	503	OLC	O20-C1	-2.41	1.26	1.33
6	B	503	PGW	O03-C01	2.13	1.49	1.45
4	B	501	OLC	O20-C21	2.28	1.50	1.45
6	B	502	PGW	O03-C01	2.32	1.50	1.45
4	A	502	OLC	O20-C21	2.36	1.50	1.45
6	B	504	PGW	O03-C01	2.38	1.50	1.45
4	A	503	OLC	O20-C21	2.53	1.50	1.45
2	B	401	1Q5	C1-C2	3.89	1.47	1.40
2	C	401	1Q5	C1-C2	3.91	1.47	1.40
2	C	401	1Q5	C15-C16	3.92	1.46	1.40
2	B	401	1Q5	C15-C16	3.98	1.46	1.40
2	A	401	1Q5	C15-C16	3.99	1.46	1.40
2	A	401	1Q5	C1-C2	4.04	1.47	1.40
2	C	401	1Q5	C1-C6	4.22	1.47	1.40
2	B	401	1Q5	C1-C6	4.31	1.47	1.40
2	A	401	1Q5	C1-C6	4.32	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	1Q5	C15-N19-C20	-3.51	119.61	125.04
2	A	401	1Q5	C14-C15-C16	-3.26	117.60	121.47
2	B	401	1Q5	C15-N19-C20	-3.21	120.07	125.04
2	C	401	1Q5	C14-C15-C16	-3.18	117.69	121.47
2	B	401	1Q5	C14-C15-C16	-3.13	117.75	121.47
2	C	401	1Q5	C15-N19-C20	-2.98	120.43	125.04
2	A	401	1Q5	C18-C13-C14	-2.21	118.30	121.82
2	B	401	1Q5	C23-C20-C21	-2.19	108.33	112.55
2	A	401	1Q5	C7-C4-C3	-2.18	117.73	120.94
2	B	401	1Q5	C7-C4-C3	-2.09	117.87	120.94
2	A	401	1Q5	C2-C1-C6	-2.05	117.70	122.14
4	A	503	OLC	O20-C1-O19	-2.04	118.48	123.55
2	C	401	1Q5	C7-C4-C3	-2.02	117.96	120.94
6	B	502	PGW	O03-C01-C02	2.25	114.31	108.66
6	B	504	PGW	O03-C19-C20	2.49	119.13	111.90
6	B	503	PGW	O03-C19-C20	2.53	119.26	111.90
4	B	501	OLC	O20-C1-C2	2.54	119.30	111.90
4	A	503	OLC	O20-C1-C2	2.55	119.33	111.90
4	A	502	OLC	O20-C1-C2	2.68	119.70	111.90
6	B	502	PGW	O03-C19-C20	2.83	120.13	111.90
2	A	401	1Q5	C3-C4-C5	3.33	122.20	118.09
2	C	401	1Q5	C3-C4-C5	3.41	122.30	118.09
2	B	401	1Q5	C3-C4-C5	3.41	122.30	118.09
2	C	401	1Q5	C1-O10-C11	3.47	120.92	116.95
2	B	401	1Q5	C1-O10-C11	3.76	121.26	116.95
6	B	502	PGW	O01-C1-C2	3.96	119.78	111.55
2	A	401	1Q5	C11-N12-C13	4.07	121.39	117.24
2	C	401	1Q5	C11-N12-C13	4.17	121.49	117.24
6	B	504	PGW	O01-C1-C2	4.28	120.43	111.55
2	B	401	1Q5	C11-N12-C13	4.29	121.61	117.24
6	B	503	PGW	O01-C1-C2	4.29	120.47	111.55
2	A	401	1Q5	C1-O10-C11	4.75	122.38	116.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	1Q5	2	0
3	A	501	OLA	1	0
4	A	502	OLC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	OLC	1	0
5	A	504	SO4	1	1
2	B	401	1Q5	5	0
4	B	501	OLC	2	0
6	B	502	PGW	4	0
6	B	503	PGW	1	0
6	B	504	PGW	5	0
5	B	506	SO4	0	1
2	C	401	1Q5	3	0
3	C	501	OLA	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	407/441 (92%)	0.25	33 (8%) 13 6	32, 56, 112, 131	0
1	B	396/441 (89%)	0.04	16 (4%) 39 22	28, 50, 92, 116	0
1	C	248/441 (56%)	0.38	27 (10%) 6 3	37, 66, 115, 139	0
All	All	1051/1323 (79%)	0.20	76 (7%) 16 8	28, 55, 109, 139	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	PRO	6.5
1	A	116	TYR	6.5
1	C	300	ALA	5.5
1	A	1054	SER	5.4
1	C	117	HIS	4.9
1	A	1053	ASN	4.7
1	C	266	VAL	4.7
1	C	148	ARG	4.5
1	C	336	GLU	4.5
1	A	1052	ARG	4.1
1	A	265	GLY	4.0
1	C	225	ARG	4.0
1	A	333	ASN	4.0
1	A	342	VAL	4.0
1	A	302	THR	3.9
1	A	340	SER	3.7
1	A	1055	ASN	3.7
1	C	253	TYR	3.7
1	C	301	SER	3.6
1	B	1044	SER	3.6
1	A	115	HIS	3.6
1	C	118	VAL	3.5
1	C	267	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	115	HIS	3.5
1	B	343	VAL	3.4
1	C	181	HIS	3.4
1	C	302	THR	3.4
1	B	1039	LEU	3.3
1	C	296	THR	3.3
1	B	267	TYR	3.2
1	B	1043	LYS	3.2
1	C	178	PRO	3.2
1	A	263	ARG	3.2
1	C	265	GLY	3.2
1	A	296	THR	3.2
1	A	264	PRO	3.1
1	C	219	LEU	3.1
1	A	346	TYR	3.1
1	A	343	VAL	3.1
1	C	179	GLU	3.0
1	A	295	MET	3.0
1	B	148	ARG	3.0
1	A	1056	GLY	3.0
1	C	182	GLN	2.9
1	B	145	ARG	2.9
1	C	183	SER	2.8
1	A	1057	VAL	2.8
1	B	1040	SER	2.7
1	B	263	ARG	2.7
1	B	1052	ARG	2.7
1	A	303	THR	2.7
1	A	267	TYR	2.7
1	C	145	ARG	2.7
1	A	117	HIS	2.7
1	C	224	ASP	2.7
1	C	177	SER	2.6
1	A	339	VAL	2.6
1	C	335	GLY	2.5
1	A	1051	GLY	2.5
1	B	1053	ASN	2.5
1	A	330	ALA	2.4
1	A	266	VAL	2.4
1	B	1056	GLY	2.4
1	A	1039	LEU	2.3
1	A	177	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	337	ASP	2.3
1	A	148	ARG	2.2
1	C	299	ARG	2.2
1	A	1026	THR	2.1
1	A	300	ALA	2.1
1	B	179	GLU	2.1
1	B	329	LEU	2.1
1	A	304	SER	2.1
1	C	143	ARG	2.1
1	B	1051	GLY	2.0
1	A	1059	THR	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	1PE	B	505	16/16	0.91	0.31	4.32	45,56,64,66	0
6	PGW	B	502	39/51	0.84	0.32	3.17	31,53,90,114	0
6	PGW	B	504	37/51	0.83	0.26	2.77	41,54,75,81	0
4	OLC	A	503	25/25	0.84	0.22	2.03	28,50,67,70	0
4	OLC	B	501	25/25	0.87	0.26	1.72	25,58,79,83	0
3	OLA	A	501	13/20	0.92	0.20	1.60	28,39,47,47	0
3	OLA	C	501	20/20	0.89	0.21	1.19	35,47,79,79	0
2	1Q5	C	401	24/24	0.94	0.21	0.96	47,52,58,69	0
2	1Q5	A	401	24/24	0.96	0.20	0.79	43,52,58,60	0
2	1Q5	B	401	24/24	0.95	0.19	0.78	35,47,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	B	508	5/5	0.93	0.17	0.70	69,80,92,103	0
6	PGW	B	503	46/51	0.86	0.26	0.60	29,49,93,111	0
4	OLC	A	502	25/25	0.89	0.19	0.03	41,53,77,82	0
5	SO4	B	507	5/5	0.99	0.18	-0.32	40,48,54,55	0
5	SO4	B	506	5/5	0.97	0.12	-1.80	62,64,72,76	0
5	SO4	A	504	5/5	0.97	0.10	-4.22	61,62,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.