



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:57 AM UTC

PDB ID : 5LYO / pdb_00005lyo
Title : Crystal structure of the zymogen matriptase catalytic domain
Authors : Hong, Z.; Jensen, J.K.
Deposited on : 2016-09-28
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

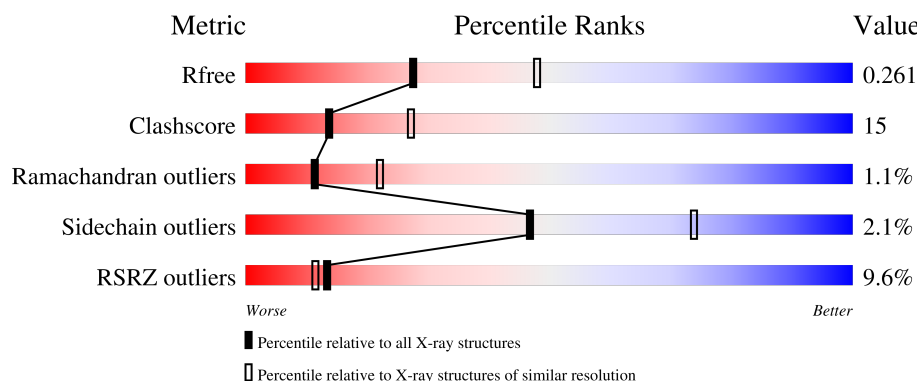
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	265	9% 71% 20% 5% • 5%
1	B	265	8% 68% 24% • 5%
1	C	265	10% 69% 23% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	904	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6136 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 Suppressor of tumorigenicity 14 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1951	1233	347	360	11			
1	B	252	Total	C	N	O	S	0	0	0
			1943	1226	346	360	11			
1	C	255	Total	C	N	O	S	0	1	0
			1970	1243	350	366	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	591	SER	-	expression tag	UNP Q9Y5Y6
A	592	MET	-	expression tag	UNP Q9Y5Y6
A	593	ASN	-	expression tag	UNP Q9Y5Y6
A	594	SER	-	expression tag	UNP Q9Y5Y6
A	595	HIS	-	expression tag	UNP Q9Y5Y6
A	596	HIS	-	expression tag	UNP Q9Y5Y6
A	597	HIS	-	expression tag	UNP Q9Y5Y6
A	598	HIS	-	expression tag	UNP Q9Y5Y6
A	599	HIS	-	expression tag	UNP Q9Y5Y6
A	600	HIS	-	expression tag	UNP Q9Y5Y6
A	601	GLY	-	expression tag	UNP Q9Y5Y6
A	602	THR	-	expression tag	UNP Q9Y5Y6
A	603	ALA	-	expression tag	UNP Q9Y5Y6
A	614	ALA	ARG	engineered mutation	UNP Q9Y5Y6
A	772	GLN	ASN	engineered mutation	UNP Q9Y5Y6
A	805	ALA	SER	engineered mutation	UNP Q9Y5Y6
B	591	SER	-	expression tag	UNP Q9Y5Y6
B	592	MET	-	expression tag	UNP Q9Y5Y6
B	593	ASN	-	expression tag	UNP Q9Y5Y6
B	594	SER	-	expression tag	UNP Q9Y5Y6
B	595	HIS	-	expression tag	UNP Q9Y5Y6
B	596	HIS	-	expression tag	UNP Q9Y5Y6
B	597	HIS	-	expression tag	UNP Q9Y5Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	598	HIS	-	expression tag	UNP Q9Y5Y6
B	599	HIS	-	expression tag	UNP Q9Y5Y6
B	600	HIS	-	expression tag	UNP Q9Y5Y6
B	601	GLY	-	expression tag	UNP Q9Y5Y6
B	602	THR	-	expression tag	UNP Q9Y5Y6
B	603	ALA	-	expression tag	UNP Q9Y5Y6
B	614	ALA	ARG	engineered mutation	UNP Q9Y5Y6
B	772	GLN	ASN	engineered mutation	UNP Q9Y5Y6
B	805	ALA	SER	engineered mutation	UNP Q9Y5Y6
C	591	SER	-	expression tag	UNP Q9Y5Y6
C	592	MET	-	expression tag	UNP Q9Y5Y6
C	593	ASN	-	expression tag	UNP Q9Y5Y6
C	594	SER	-	expression tag	UNP Q9Y5Y6
C	595	HIS	-	expression tag	UNP Q9Y5Y6
C	596	HIS	-	expression tag	UNP Q9Y5Y6
C	597	HIS	-	expression tag	UNP Q9Y5Y6
C	598	HIS	-	expression tag	UNP Q9Y5Y6
C	599	HIS	-	expression tag	UNP Q9Y5Y6
C	600	HIS	-	expression tag	UNP Q9Y5Y6
C	601	GLY	-	expression tag	UNP Q9Y5Y6
C	602	THR	-	expression tag	UNP Q9Y5Y6
C	603	ALA	-	expression tag	UNP Q9Y5Y6
C	614	ALA	ARG	engineered mutation	UNP Q9Y5Y6
C	772	GLN	ASN	engineered mutation	UNP Q9Y5Y6
C	805	ALA	SER	engineered mutation	UNP Q9Y5Y6

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

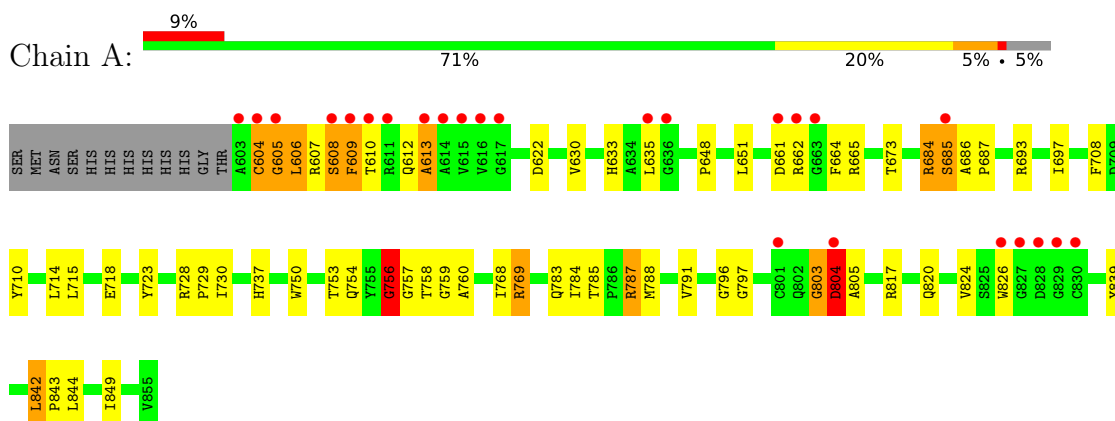
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	60	Total 60	O 60	0	0
3	C	52	Total 52	O 52	0	0

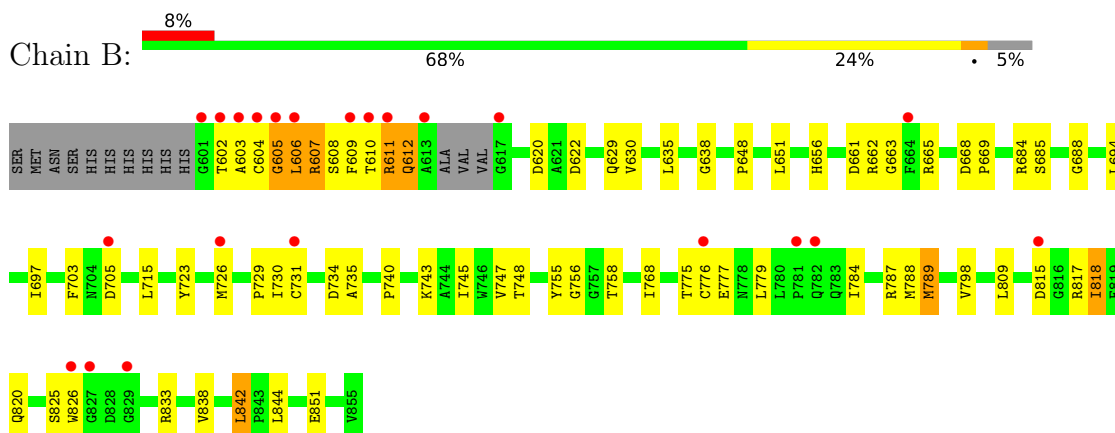
3 Residue-property plots [i](#)

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.

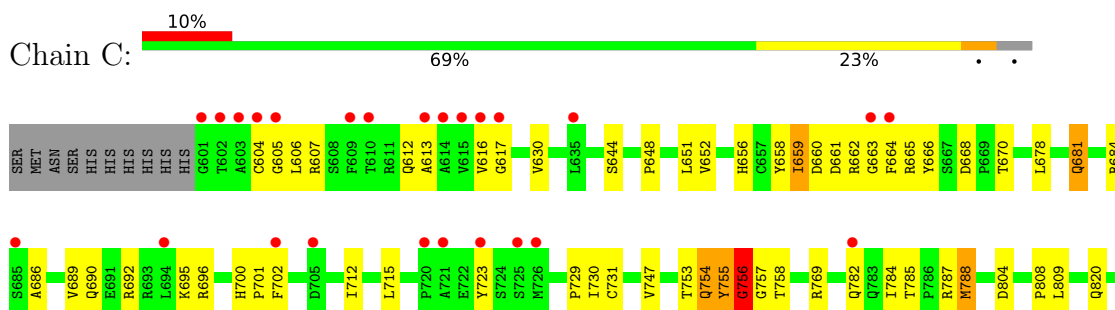
- Molecule 1: Suppressor of tumorigenicity 14 protein

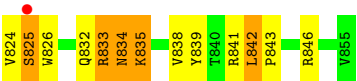


- Molecule 1: Suppressor of tumorigenicity 14 protein



- Molecule 1: Suppressor of tumorigenicity 14 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.17Å 109.17Å 124.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.27 – 2.50 47.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.27-2.50) 98.8 (47.27-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.214 , 0.263 0.215 , 0.261	Depositor DCC
R_{free} test set	1494 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6136	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4349e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.67	1/2004 (0.0%)	1.44	24/2725 (0.9%)
1	B	0.59	1/1995 (0.1%)	0.80	11/2710 (0.4%)
1	C	0.69	4/2023 (0.2%)	1.23	21/2751 (0.8%)
All	All	0.65	6/6022 (0.1%)	1.19	56/8186 (0.7%)

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	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	685	SER	C-N	-8.09	1.22	1.33
1	C	835	LYS	C-O	-6.37	1.18	1.24
1	C	835	LYS	CA-C	-5.88	1.46	1.52
1	B	818	ILE	C-O	-5.65	1.17	1.24
1	C	788	MET	C-O	-5.34	1.17	1.24
1	C	835	LYS	N-CA	-5.20	1.41	1.45

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	SER	CA-C-N	34.84	173.91	120.60
1	A	685	SER	C-N-CA	34.84	173.91	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	612	GLN	N-CA-C	24.93	145.65	111.24
1	C	613	ALA	N-CA-C	24.25	137.94	111.03
1	A	685	SER	N-CA-C	23.20	141.92	113.16
1	C	612	GLN	CB-CA-C	-18.32	83.88	112.09
1	A	685	SER	CB-CA-C	-15.74	81.68	110.01
1	C	825	SER	N-CA-C	15.33	132.87	113.55
1	A	804	ASP	CB-CA-C	13.70	136.13	110.10
1	C	826	TRP	N-CA-C	-12.87	87.02	108.76
1	C	613	ALA	N-CA-CB	-12.49	91.87	109.98
1	C	617	GLY	N-CA-C	12.17	128.43	112.13
1	C	684	ARG	N-CA-C	-10.41	98.00	113.61
1	B	825	SER	N-CA-C	10.38	126.48	112.68
1	B	826	TRP	N-CA-C	-9.41	94.43	109.59
1	C	607	ARG	N-CA-C	9.18	123.17	109.95
1	B	612	GLN	N-CA-C	8.96	123.05	108.99
1	A	804	ASP	N-CA-C	-8.89	86.09	111.00
1	A	606	LEU	N-CA-CB	-8.72	96.55	110.77
1	A	805	ALA	N-CA-C	-8.70	94.71	109.24
1	C	825	SER	CB-CA-C	-8.60	96.02	109.34
1	A	684	ARG	N-CA-C	-8.43	103.14	113.50
1	A	687	PRO	N-CA-C	7.92	124.54	113.53
1	A	685	SER	O-C-N	-7.73	111.70	122.37
1	B	825	SER	CB-CA-C	-7.50	97.71	110.24
1	A	686	ALA	N-CA-C	-7.41	99.53	109.84
1	A	756	GLY	N-CA-C	7.39	130.70	113.18
1	C	756	GLY	N-CA-C	7.36	130.61	113.18
1	A	605	GLY	N-CA-C	7.29	130.47	113.18
1	A	803	GLY	CA-C-O	-7.12	115.09	121.64
1	C	616	VAL	CB-CA-C	-7.06	99.72	111.29
1	C	834	ASN	N-CA-C	7.05	119.05	111.36
1	A	613	ALA	N-CA-C	-6.90	97.82	108.31
1	A	817	ARG	CG-CD-NE	6.85	127.07	112.00
1	B	776	CYS	CA-CB-SG	-6.63	99.15	114.40
1	A	803	GLY	CA-C-N	6.34	133.11	121.70
1	A	803	GLY	C-N-CA	6.34	133.11	121.70
1	B	798	VAL	N-CA-C	-6.33	107.08	113.47
1	B	684	ARG	N-CA-C	-6.19	105.67	113.72
1	A	803	GLY	N-CA-C	-6.17	101.96	111.64
1	A	686	ALA	N-CA-CB	5.94	119.00	110.03
1	C	834	ASN	CB-CA-C	-5.94	100.75	110.85
1	B	755	TYR	N-CA-C	5.87	119.75	112.59
1	B	758	THR	N-CA-C	5.81	118.91	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	835	LYS	N-CA-C	5.79	117.59	108.55
1	C	826	TRP	N-CA-CB	5.78	120.80	110.80
1	C	833	ARG	CA-C-N	5.39	127.94	120.29
1	C	833	ARG	C-N-CA	5.39	127.94	120.29
1	A	606	LEU	N-CA-C	-5.28	99.50	108.26
1	A	787	ARG	CA-CB-CG	-5.17	103.75	114.10
1	A	604	CYS	O-C-N	-5.08	116.40	122.65
1	C	835	LYS	N-CA-CB	-5.08	102.04	111.18
1	C	754	GLN	N-CA-C	-5.07	103.79	110.33
1	B	610	THR	N-CA-C	5.06	119.41	112.68
1	B	756	GLY	N-CA-C	5.04	120.69	114.69
1	C	788	MET	N-CA-C	5.01	117.66	109.59

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	604	CYS	Mainchain
1	A	685	SER	Mainchain
1	A	756	GLY	Peptide
1	B	605	GLY	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	1951	0	1869	49	2
1	B	1943	0	1858	62	0
1	C	1970	0	1883	60	2
2	A	35	0	0	2	0
2	B	25	0	0	4	0
2	C	45	0	0	1	0
3	A	55	0	0	0	0
3	B	60	0	0	6	0
3	C	52	0	0	1	0
All	All	6136	0	5610	168	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (168) 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:604:CYS:SG	1:B:731:CYS:SG	1.48	1.46
1:B:606:LEU:O	3:B:1001:HOH:O	1.67	1.08
1:C:785:THR:H	1:C:788:MET:HE2	0.90	1.07
1:C:785:THR:N	1:C:788:MET:HE2	1.73	1.04
1:B:606:LEU:O	1:B:607:ARG:HG3	1.59	1.03
1:B:851:GLU:OE2	3:B:1002:HOH:O	1.79	0.99
1:B:602:THR:HG21	3:B:1050:HOH:O	1.63	0.98
1:A:787:ARG:HG2	1:A:844:LEU:HD11	1.44	0.97
1:C:784:ILE:HA	1:C:788:MET:CE	1.95	0.96
1:C:784:ILE:HA	1:C:788:MET:HE1	1.50	0.94
1:B:611:ARG:NH1	3:B:1003:HOH:O	1.89	0.89
1:A:803:GLY:HA2	1:A:804:ASP:HB2	1.57	0.85
1:C:604:CYS:O	1:C:731:CYS:SG	2.35	0.84
1:B:605:GLY:HA3	1:B:606:LEU:HD13	1.64	0.79
1:A:784:ILE:HA	1:A:788:MET:CE	2.13	0.78
1:B:606:LEU:O	1:B:607:ARG:CG	2.32	0.77
1:C:785:THR:H	1:C:788:MET:CE	1.86	0.76
1:A:785:THR:H	1:A:788:MET:HE2	1.47	0.76
1:B:603:ALA:C	1:B:729:PRO:HG2	2.11	0.75
1:A:804:ASP:O	1:A:824:VAL:HG11	1.86	0.75
1:C:656:HIS:CE1	1:C:825:SER:O	2.41	0.73
1:B:784:ILE:HA	1:B:788:MET:HE2	1.71	0.73
1:C:782:GLN:NE2	3:C:1001:HOH:O	2.21	0.72
1:B:603:ALA:CB	1:B:723:TYR:CE2	2.73	0.72
1:C:754:GLN:C	1:C:756:GLY:H	1.98	0.71
1:C:662:ARG:HD2	1:C:663:GLY:H	1.59	0.68
1:B:604:CYS:SG	1:B:605:GLY:N	2.62	0.67
1:B:685:SER:OG	3:B:1005:HOH:O	2.11	0.67
2:B:904:SO4:O2	3:B:1004:HOH:O	2.11	0.67
1:B:611:ARG:O	1:B:612:GLN:HG2	1.96	0.66
1:B:669:PRO:HB3	1:B:697:ILE:HG13	1.78	0.66
1:B:694:LEU:HD21	1:B:715:LEU:HD13	1.76	0.66
1:B:604:CYS:O	1:B:606:LEU:HB2	1.97	0.65
1:C:605:GLY:N	1:C:729:PRO:O	2.25	0.65
1:A:693:ARG:NH2	1:B:668:ASP:OD2	2.30	0.64
1:C:700:HIS:HE1	1:C:702:PHE:HD2	1.46	0.64
1:C:754:GLN:C	1:C:756:GLY:N	2.54	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:ARG:HG3	1:B:663:GLY:H	1.63	0.62
1:A:635:LEU:HB3	1:B:635:LEU:HB3	1.82	0.62
1:C:804[B]:ASP:OD1	1:C:804[B]:ASP:N	2.21	0.62
1:B:611:ARG:C	1:B:612:GLN:HG2	2.23	0.62
1:B:603:ALA:O	1:B:729:PRO:HG2	2.00	0.61
1:C:754:GLN:O	1:C:756:GLY:N	2.33	0.61
1:A:785:THR:N	1:A:788:MET:HE2	2.17	0.59
1:C:820:GLN:HG2	1:C:842:LEU:HD22	1.85	0.59
1:B:605:GLY:O	1:B:818:ILE:N	2.24	0.58
1:A:737:HIS:ND1	2:A:903:SO4:O3	2.32	0.58
1:C:700:HIS:CE1	1:C:702:PHE:HD2	2.21	0.57
1:B:606:LEU:O	1:B:607:ARG:CB	2.52	0.57
1:C:661:ASP:O	1:C:662:ARG:HG3	2.05	0.57
1:C:747:VAL:HG22	1:C:809:LEU:HD22	1.87	0.57
1:C:730:ILE:HD13	1:C:820:GLN:HB2	1.88	0.56
1:B:606:LEU:C	1:B:607:ARG:CG	2.78	0.56
1:B:661:ASP:O	1:B:662:ARG:HG2	2.05	0.56
1:B:603:ALA:CB	1:B:723:TYR:HE2	2.17	0.56
1:A:718:GLU:OE1	1:B:665:ARG:NH2	2.39	0.56
1:B:606:LEU:C	1:B:607:ARG:HG3	2.29	0.56
1:B:656:HIS:HE1	2:B:901:SO4:O3	1.88	0.56
1:B:608:SER:OG	1:B:609:PHE:N	2.38	0.55
1:C:695:LYS:HG2	1:C:696:ARG:HG3	1.87	0.55
1:A:820:GLN:HG2	1:A:842:LEU:HD22	1.88	0.55
1:A:783:GLN:O	1:A:788:MET:HE1	2.06	0.55
1:A:608:SER:OG	1:A:728:ARG:NH1	2.40	0.55
1:B:777:GLU:HA	1:B:784:ILE:HG21	1.89	0.55
1:A:784:ILE:HA	1:A:788:MET:HE3	1.87	0.54
1:B:648:PRO:HD3	1:B:723:TYR:OH	2.07	0.54
1:C:754:GLN:O	1:C:755:TYR:CG	2.60	0.54
1:A:609:PHE:HE2	1:A:612:GLN:OE1	1.89	0.54
1:A:697:ILE:HD13	1:A:715:LEU:HG	1.89	0.54
1:A:730:ILE:HD13	1:A:820:GLN:HB2	1.91	0.54
1:B:662:ARG:HG3	1:B:663:GLY:N	2.22	0.53
1:B:638:GLY:N	2:B:902:SO4:O1	2.39	0.53
1:B:629:GLN:OE1	1:B:748:THR:HG23	2.09	0.53
1:C:832:GLN:HE21	1:C:834:ASN:HB2	1.72	0.53
1:C:755:TYR:C	1:C:755:TYR:CD1	2.86	0.53
1:B:612:GLN:OE1	1:B:622:ASP:HB2	2.09	0.52
1:C:665:ARG:O	1:C:665:ARG:HG3	2.10	0.52
1:B:820:GLN:HG2	1:B:842:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:HIS:HB2	1:C:712:ILE:HG23	1.89	0.52
1:A:710:TYR:CZ	1:A:787:ARG:CD	2.93	0.52
1:A:633:HIS:CE1	1:A:684:ARG:HH12	2.28	0.52
1:C:668:ASP:OD2	1:C:670:THR:OG1	2.27	0.52
1:A:708:PHE:HD2	1:A:826:TRP:CD1	2.28	0.51
1:A:784:ILE:HA	1:A:788:MET:HE2	1.91	0.51
1:A:633:HIS:CE1	1:A:684:ARG:NH1	2.78	0.51
1:B:603:ALA:HB3	1:B:723:TYR:CE2	2.46	0.51
1:A:605:GLY:N	1:A:729:PRO:O	2.42	0.51
1:A:648:PRO:HD3	1:A:723:TYR:OH	2.10	0.51
1:C:630:VAL:HG21	1:C:651:LEU:HD22	1.93	0.51
1:B:747:VAL:HG22	1:B:809:LEU:HD22	1.93	0.50
1:A:758:THR:HG22	1:A:759:GLY:O	2.13	0.49
1:A:718:GLU:CD	1:B:665:ARG:HH22	2.19	0.49
1:C:769:ARG:O	1:C:769:ARG:HG3	2.13	0.48
1:B:603:ALA:HB3	1:B:723:TYR:HE2	1.78	0.48
1:B:661:ASP:OD1	1:B:662:ARG:N	2.47	0.48
1:B:605:GLY:HA2	1:B:817:ARG:HB3	1.96	0.48
1:A:609:PHE:CG	1:A:609:PHE:O	2.66	0.48
1:A:661:ASP:OD1	1:A:662:ARG:N	2.46	0.48
1:C:692:ARG:NH1	2:C:908:SO4:O4	2.47	0.48
1:C:659:ILE:O	1:C:659:ILE:HG13	2.14	0.47
1:B:688:GLY:HA3	1:B:726:MET:SD	2.55	0.47
1:A:750:TRP:HD1	1:A:760:ALA:O	1.97	0.47
1:A:842:LEU:H	1:A:843:PRO:CD	2.28	0.47
1:B:703:PHE:CE2	1:B:705:ASP:HB2	2.49	0.47
1:C:644:SER:HB3	1:C:808:PRO:HB3	1.95	0.47
1:C:648:PRO:HD3	1:C:723:TYR:OH	2.15	0.46
1:C:846:ARG:O	1:C:846:ARG:HD2	2.15	0.46
1:B:734:ASP:OD1	1:B:735:ALA:N	2.49	0.46
1:C:824:VAL:HA	1:C:839:TYR:HD2	1.81	0.46
1:C:784:ILE:HD12	1:C:838:VAL:HG11	1.96	0.46
1:C:753:THR:OG1	1:C:754:GLN:O	2.30	0.45
1:A:609:PHE:CE2	1:A:612:GLN:OE1	2.69	0.45
1:A:710:TYR:CE2	1:A:787:ARG:NE	2.85	0.45
1:A:630:VAL:HG21	1:A:651:LEU:HD22	1.98	0.45
1:C:723:TYR:OH	1:C:729:PRO:HG3	2.17	0.45
1:A:804:ASP:O	1:A:824:VAL:CG1	2.62	0.45
1:A:803:GLY:CA	1:A:804:ASP:HB2	2.38	0.45
1:C:784:ILE:CA	1:C:788:MET:CE	2.83	0.45
1:C:658:TYR:OH	1:C:715:LEU:HD11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:CYS:C	1:C:731:CYS:SG	2.99	0.45
1:C:678:LEU:HD21	1:C:681:GLN:NE2	2.32	0.45
1:A:753:THR:OG1	1:A:757:GLY:HA3	2.17	0.44
1:A:824:VAL:HA	1:A:839:TYR:HD2	1.82	0.44
1:C:753:THR:OG1	1:C:757:GLY:HA3	2.17	0.44
1:A:635:LEU:HA	2:A:902:SO4:O4	2.17	0.44
1:C:755:TYR:CD1	1:C:755:TYR:O	2.70	0.44
1:A:664:PHE:HD1	1:A:665:ARG:N	2.16	0.44
1:B:740:PRO:HD2	1:B:743:LYS:HB2	2.00	0.44
1:C:700:HIS:CE1	1:C:702:PHE:CD2	3.04	0.44
1:B:730:ILE:HG12	1:B:731:CYS:N	2.33	0.44
1:C:656:HIS:HE1	1:C:825:SER:O	1.96	0.44
1:C:755:TYR:O	1:C:755:TYR:HD1	2.01	0.44
1:B:833:ARG:NH1	2:B:904:SO4:O4	2.48	0.44
1:C:842:LEU:H	1:C:843:PRO:CD	2.31	0.43
1:A:768:ILE:HD12	1:A:768:ILE:C	2.43	0.43
1:B:789:MET:HE2	1:B:789:MET:HB3	1.79	0.43
1:C:686:ALA:HB3	1:C:689:VAL:HG23	2.00	0.43
1:A:609:PHE:O	1:A:609:PHE:CD1	2.70	0.43
1:B:775:THR:O	1:B:779:LEU:HD13	2.18	0.43
1:C:787:ARG:O	1:C:841:ARG:HG3	2.18	0.43
1:B:787:ARG:HG3	1:B:844:LEU:HD11	1.99	0.43
1:A:769:ARG:O	1:A:769:ARG:HG3	2.16	0.43
1:A:796:GLY:HA3	1:A:797:GLY:HA3	1.73	0.42
1:B:606:LEU:HD12	1:B:606:LEU:HA	1.87	0.42
1:C:701:PRO:HG2	1:C:702:PHE:CE2	2.54	0.42
1:C:652:VAL:HG13	1:C:712:ILE:HD11	2.01	0.42
1:C:753:THR:C	1:C:754:GLN:O	2.60	0.42
1:A:768:ILE:HD13	1:A:791:VAL:HB	2.01	0.42
1:B:788:MET:HE3	1:B:838:VAL:HG11	2.02	0.42
1:C:664:PHE:HD1	1:C:665:ARG:N	2.18	0.42
1:A:633:HIS:HE1	1:A:684:ARG:NH1	2.16	0.42
1:B:815:ASP:OD1	1:B:815:ASP:C	2.62	0.42
1:C:835:LYS:HE3	1:C:835:LYS:HB2	1.86	0.42
1:A:714:LEU:HD21	1:A:849:ILE:HG12	2.01	0.41
1:B:630:VAL:HG21	1:B:651:LEU:HD22	2.03	0.41
1:A:826:TRP:CD1	1:A:826:TRP:H	2.39	0.41
1:B:611:ARG:HD3	1:B:611:ARG:HA	1.73	0.41
1:B:620:ASP:N	1:B:620:ASP:OD1	2.54	0.41
1:B:745:ILE:HB	1:B:768:ILE:HD11	2.03	0.41
1:C:756:GLY:HA2	1:C:757:GLY:HA3	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:PHE:CD1	1:C:664:PHE:C	2.99	0.41
1:B:730:ILE:HD13	1:B:820:GLN:HB2	2.04	0.40
1:A:613:ALA:HB3	1:A:622:ASP:OD2	2.20	0.40
1:B:705:ASP:O	1:B:705:ASP:CG	2.64	0.40
1:A:635:LEU:HD11	1:A:673:THR:OG1	2.22	0.40
1:C:660:ASP:OD1	1:C:666:TYR:N	2.54	0.40
1:C:690:GLN:OE1	1:C:692:ARG:NH2	2.54	0.40
1:C:662:ARG:CD	1:C:663:GLY:H	2.32	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:GLN:OE1	1:C:833:ARG:NH1[3_544]	2.18	0.02
1:A:758:THR:O	1:C:769:ARG:NH1[3_544]	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	251/265 (95%)	238 (95%)	10 (4%)	3 (1%)	10	20
1	B	248/265 (94%)	235 (95%)	11 (4%)	2 (1%)	16	31
1	C	254/265 (96%)	238 (94%)	13 (5%)	3 (1%)	10	20
All	All	753/795 (95%)	711 (94%)	34 (4%)	8 (1%)	11	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	755	TYR
1	B	607	ARG
1	C	756	GLY

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Mol	Chain	Res	Type
1	A	804	ASP
1	A	756	GLY
1	A	842	LEU
1	B	842	LEU
1	C	842	LEU

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	204/215 (95%)	198 (97%)	6 (3%)	37	65
1	B	203/215 (94%)	200 (98%)	3 (2%)	57	80
1	C	206/215 (96%)	202 (98%)	4 (2%)	50	76
All	All	613/645 (95%)	600 (98%)	13 (2%)	47	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	606	LEU
1	A	607	ARG
1	A	608	SER
1	A	609	PHE
1	A	610	THR
1	A	769	ARG
1	B	606	LEU
1	B	611	ARG
1	B	789	MET
1	C	606	LEU
1	C	659	ILE
1	C	681	GLN
1	C	758	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	773	GLN
1	B	637	GLN
1	C	637	GLN
1	C	754	GLN
1	C	832	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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	SO4	C	904	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	903	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	901	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	903	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	C	901	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	907	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	A	904	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	C	905	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	C	907	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	901	-	4,4,4	0.24	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	904	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	902	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	B	905	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	903	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	906	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	906	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	902	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	C	902	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	C	908	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	905	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	C	909	-	4,4,4	0.24	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	SO4	1	0
2	A	903	SO4	1	0
2	B	904	SO4	2	0
2	B	902	SO4	1	0
2	A	902	SO4	1	0
2	C	908	SO4	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	253/265 (95%)	0.37	25 (9%)	13 11	24, 41, 89, 163	0
1	B	252/265 (95%)	0.44	22 (8%)	16 14	26, 42, 85, 124	0
1	C	255/265 (96%)	0.67	26 (10%)	12 10	20, 47, 93, 189	1 (0%)
All	All	760/795 (95%)	0.49	73 (9%)	13 11	20, 43, 89, 189	1 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	603	ALA	9.6
1	C	614	ALA	7.8
1	A	616	VAL	5.5
1	B	604	CYS	5.4
1	C	616	VAL	5.4
1	A	826	TRP	5.2
1	A	827	GLY	5.2
1	A	610	THR	4.8
1	A	609	PHE	4.4
1	C	613	ALA	4.4
1	C	615	VAL	4.2
1	C	702	PHE	4.2
1	A	804	ASP	4.1
1	C	602	THR	4.0
1	A	613	ALA	3.9
1	B	705	ASP	3.9
1	A	615	VAL	3.8
1	C	723	TYR	3.8
1	A	614	ALA	3.6
1	B	815	ASP	3.6
1	B	826	TRP	3.6
1	B	609	PHE	3.6
1	C	725	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	617	GLY	3.4
1	B	605	GLY	3.3
1	A	685	SER	3.3
1	A	635	LEU	3.2
1	B	613	ALA	3.1
1	B	601	GLY	3.1
1	B	776	CYS	3.0
1	A	636	GLY	2.9
1	A	617	GLY	2.8
1	B	611	ARG	2.8
1	B	602	THR	2.8
1	C	610	THR	2.8
1	C	604	CYS	2.8
1	C	617	GLY	2.8
1	A	603	ALA	2.8
1	A	662	ARG	2.6
1	A	605	GLY	2.6
1	B	827	GLY	2.6
1	C	685	SER	2.6
1	C	603	ALA	2.5
1	B	781	PRO	2.5
1	A	828	ASP	2.5
1	C	605	GLY	2.5
1	B	606	LEU	2.5
1	C	664	PHE	2.5
1	C	705	ASP	2.5
1	C	782	GLN	2.5
1	B	782	GLN	2.5
1	A	611	ARG	2.4
1	B	829	GLY	2.4
1	C	663	GLY	2.4
1	C	601	GLY	2.4
1	A	830	CYS	2.3
1	A	604	CYS	2.2
1	A	608	SER	2.2
1	C	720	PRO	2.2
1	C	825	SER	2.2
1	C	609	PHE	2.2
1	B	726	MET	2.1
1	C	721	ALA	2.1
1	A	663	GLY	2.1
1	B	610	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	726	MET	2.1
1	C	635	LEU	2.1
1	A	829	GLY	2.1
1	A	661	ASP	2.1
1	C	694	LEU	2.0
1	A	801	CYS	2.0
1	B	731	CYS	2.0
1	B	664	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	906	5/5	0.64	0.16	100,103,107,109	0
2	SO4	C	909	5/5	0.64	0.14	145,146,146,148	0
2	SO4	C	902	5/5	0.67	0.16	126,127,128,128	0
2	SO4	C	908	5/5	0.72	0.12	119,119,120,120	0
2	SO4	C	904	5/5	0.78	0.14	106,109,110,112	0
2	SO4	C	906	5/5	0.78	0.15	106,108,110,114	0
2	SO4	A	904	5/5	0.79	0.19	134,135,136,137	0
2	SO4	C	903	5/5	0.81	0.15	112,115,116,116	0
2	SO4	A	901	5/5	0.82	0.12	92,95,99,99	0
2	SO4	A	903	5/5	0.83	0.12	104,108,109,113	0
2	SO4	A	907	5/5	0.83	0.16	119,120,123,124	0
2	SO4	C	907	5/5	0.84	0.17	125,127,129,130	0
2	SO4	A	902	5/5	0.84	0.14	91,99,101,102	0
2	SO4	B	905	5/5	0.84	0.12	86,93,97,97	0
2	SO4	B	904	5/5	0.85	0.14	88,90,93,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	902	5/5	0.86	0.15	80,87,89,93	0
2	SO4	B	901	5/5	0.87	0.11	88,93,95,99	0
2	SO4	C	901	5/5	0.88	0.12	101,104,108,109	0
2	SO4	B	903	5/5	0.88	0.10	93,99,101,105	0
2	SO4	A	905	5/5	0.89	0.15	82,86,87,91	0
2	SO4	C	905	5/5	0.99	0.06	26,28,36,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.