



Full wwPDB X-ray Structure Validation Report i

Aug 9, 2021 – 01:03 pm BST

PDB ID : 7A0A
Title : Crystal structure of mouse CSAD in apo form
Authors : Mahootchi, E.; Raasakka, A.; Haavik, J.; Kursula, P.
Deposited on : 2020-08-07
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.1.3
EDS : 2.23.1
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) : 2.23.1

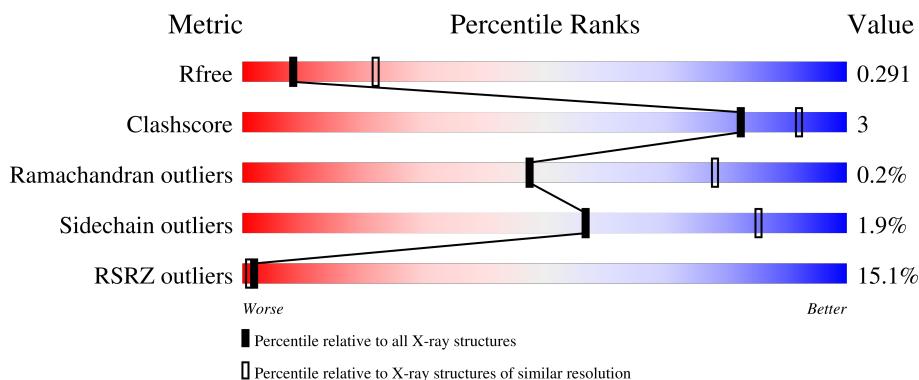
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29915 atoms, of which 14975 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 Cysteine sulfenic acid decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	474	Total	C 7486	H 2375	N 3750	O 656	S 684	21	0	0
1	B	470	Total	C 7415	H 2355	N 3716	O 647	S 676	21	0	0
1	C	478	Total	C 7524	H 2386	N 3768	O 660	S 689	21	0	0
1	D	473	Total	C 7462	H 2367	N 3741	O 653	S 680	21	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q9DBE0
A	-26	GLY	-	expression tag	UNP Q9DBE0
A	-25	PRO	-	expression tag	UNP Q9DBE0
A	-24	HIS	-	expression tag	UNP Q9DBE0
A	-23	HIS	-	expression tag	UNP Q9DBE0
A	-22	HIS	-	expression tag	UNP Q9DBE0
A	-21	HIS	-	expression tag	UNP Q9DBE0
A	-20	HIS	-	expression tag	UNP Q9DBE0
A	-19	HIS	-	expression tag	UNP Q9DBE0
A	-18	LEU	-	expression tag	UNP Q9DBE0
A	-17	GLU	-	expression tag	UNP Q9DBE0
A	-16	SER	-	expression tag	UNP Q9DBE0
A	-15	THR	-	expression tag	UNP Q9DBE0
A	-14	SER	-	expression tag	UNP Q9DBE0
A	-13	LEU	-	expression tag	UNP Q9DBE0
A	-12	TYR	-	expression tag	UNP Q9DBE0
A	-11	LYS	-	expression tag	UNP Q9DBE0
A	-10	LYS	-	expression tag	UNP Q9DBE0
A	-9	ALA	-	expression tag	UNP Q9DBE0
A	-8	GLY	-	expression tag	UNP Q9DBE0
A	-7	SER	-	expression tag	UNP Q9DBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLU	-	expression tag	UNP Q9DBE0
A	-5	ASN	-	expression tag	UNP Q9DBE0
A	-4	LEU	-	expression tag	UNP Q9DBE0
A	-3	TYR	-	expression tag	UNP Q9DBE0
A	-2	PHE	-	expression tag	UNP Q9DBE0
A	-1	GLN	-	expression tag	UNP Q9DBE0
A	0	GLY	-	expression tag	UNP Q9DBE0
B	-27	MET	-	initiating methionine	UNP Q9DBE0
B	-26	GLY	-	expression tag	UNP Q9DBE0
B	-25	PRO	-	expression tag	UNP Q9DBE0
B	-24	HIS	-	expression tag	UNP Q9DBE0
B	-23	HIS	-	expression tag	UNP Q9DBE0
B	-22	HIS	-	expression tag	UNP Q9DBE0
B	-21	HIS	-	expression tag	UNP Q9DBE0
B	-20	HIS	-	expression tag	UNP Q9DBE0
B	-19	HIS	-	expression tag	UNP Q9DBE0
B	-18	LEU	-	expression tag	UNP Q9DBE0
B	-17	GLU	-	expression tag	UNP Q9DBE0
B	-16	SER	-	expression tag	UNP Q9DBE0
B	-15	THR	-	expression tag	UNP Q9DBE0
B	-14	SER	-	expression tag	UNP Q9DBE0
B	-13	LEU	-	expression tag	UNP Q9DBE0
B	-12	TYR	-	expression tag	UNP Q9DBE0
B	-11	LYS	-	expression tag	UNP Q9DBE0
B	-10	LYS	-	expression tag	UNP Q9DBE0
B	-9	ALA	-	expression tag	UNP Q9DBE0
B	-8	GLY	-	expression tag	UNP Q9DBE0
B	-7	SER	-	expression tag	UNP Q9DBE0
B	-6	GLU	-	expression tag	UNP Q9DBE0
B	-5	ASN	-	expression tag	UNP Q9DBE0
B	-4	LEU	-	expression tag	UNP Q9DBE0
B	-3	TYR	-	expression tag	UNP Q9DBE0
B	-2	PHE	-	expression tag	UNP Q9DBE0
B	-1	GLN	-	expression tag	UNP Q9DBE0
B	0	GLY	-	expression tag	UNP Q9DBE0
C	-27	MET	-	initiating methionine	UNP Q9DBE0
C	-26	GLY	-	expression tag	UNP Q9DBE0
C	-25	PRO	-	expression tag	UNP Q9DBE0
C	-24	HIS	-	expression tag	UNP Q9DBE0
C	-23	HIS	-	expression tag	UNP Q9DBE0
C	-22	HIS	-	expression tag	UNP Q9DBE0
C	-21	HIS	-	expression tag	UNP Q9DBE0

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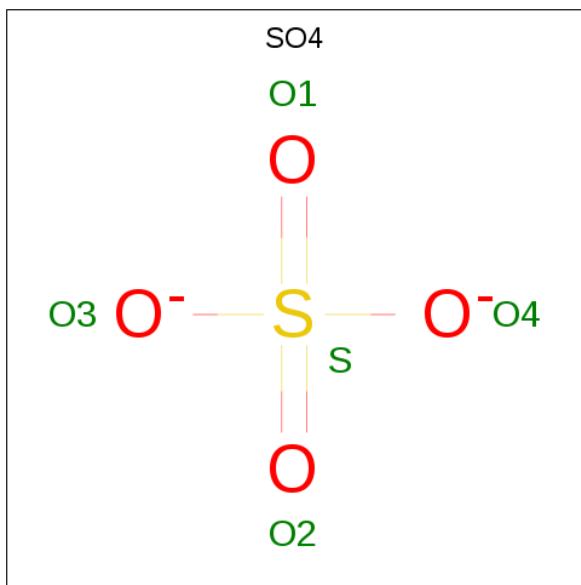
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q9DBE0
C	-19	HIS	-	expression tag	UNP Q9DBE0
C	-18	LEU	-	expression tag	UNP Q9DBE0
C	-17	GLU	-	expression tag	UNP Q9DBE0
C	-16	SER	-	expression tag	UNP Q9DBE0
C	-15	THR	-	expression tag	UNP Q9DBE0
C	-14	SER	-	expression tag	UNP Q9DBE0
C	-13	LEU	-	expression tag	UNP Q9DBE0
C	-12	TYR	-	expression tag	UNP Q9DBE0
C	-11	LYS	-	expression tag	UNP Q9DBE0
C	-10	LYS	-	expression tag	UNP Q9DBE0
C	-9	ALA	-	expression tag	UNP Q9DBE0
C	-8	GLY	-	expression tag	UNP Q9DBE0
C	-7	SER	-	expression tag	UNP Q9DBE0
C	-6	GLU	-	expression tag	UNP Q9DBE0
C	-5	ASN	-	expression tag	UNP Q9DBE0
C	-4	LEU	-	expression tag	UNP Q9DBE0
C	-3	TYR	-	expression tag	UNP Q9DBE0
C	-2	PHE	-	expression tag	UNP Q9DBE0
C	-1	GLN	-	expression tag	UNP Q9DBE0
C	0	GLY	-	expression tag	UNP Q9DBE0
D	-27	MET	-	initiating methionine	UNP Q9DBE0
D	-26	GLY	-	expression tag	UNP Q9DBE0
D	-25	PRO	-	expression tag	UNP Q9DBE0
D	-24	HIS	-	expression tag	UNP Q9DBE0
D	-23	HIS	-	expression tag	UNP Q9DBE0
D	-22	HIS	-	expression tag	UNP Q9DBE0
D	-21	HIS	-	expression tag	UNP Q9DBE0
D	-20	HIS	-	expression tag	UNP Q9DBE0
D	-19	HIS	-	expression tag	UNP Q9DBE0
D	-18	LEU	-	expression tag	UNP Q9DBE0
D	-17	GLU	-	expression tag	UNP Q9DBE0
D	-16	SER	-	expression tag	UNP Q9DBE0
D	-15	THR	-	expression tag	UNP Q9DBE0
D	-14	SER	-	expression tag	UNP Q9DBE0
D	-13	LEU	-	expression tag	UNP Q9DBE0
D	-12	TYR	-	expression tag	UNP Q9DBE0
D	-11	LYS	-	expression tag	UNP Q9DBE0
D	-10	LYS	-	expression tag	UNP Q9DBE0
D	-9	ALA	-	expression tag	UNP Q9DBE0
D	-8	GLY	-	expression tag	UNP Q9DBE0
D	-7	SER	-	expression tag	UNP Q9DBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLU	-	expression tag	UNP Q9DBE0
D	-5	ASN	-	expression tag	UNP Q9DBE0
D	-4	LEU	-	expression tag	UNP Q9DBE0
D	-3	TYR	-	expression tag	UNP Q9DBE0
D	-2	PHE	-	expression tag	UNP Q9DBE0
D	-1	GLN	-	expression tag	UNP Q9DBE0
D	0	GLY	-	expression tag	UNP Q9DBE0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

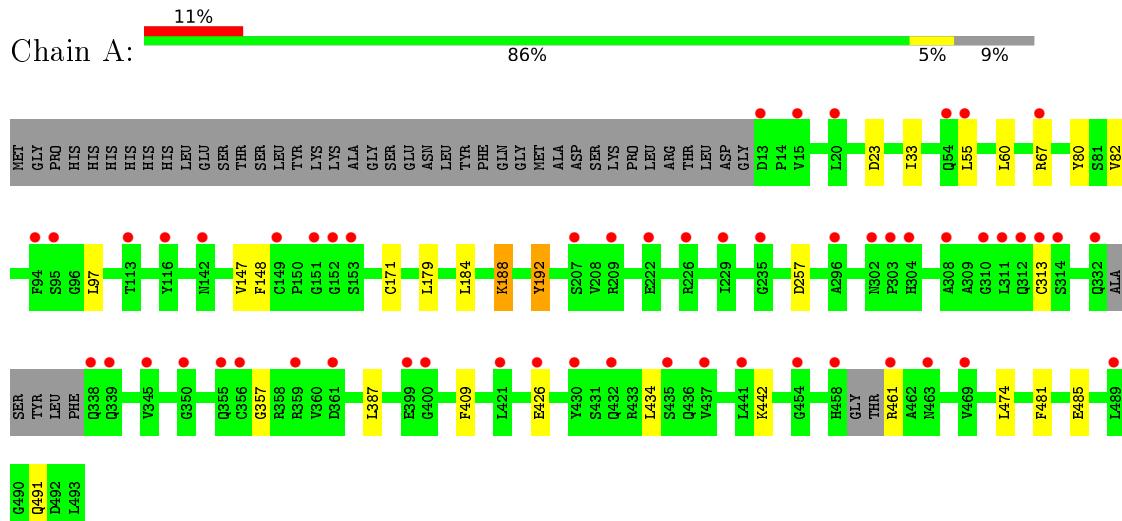
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	4	Total O 4 4	0	0
4	C	9	Total O 9 9	0	0
4	D	2	Total O 2 2	0	0

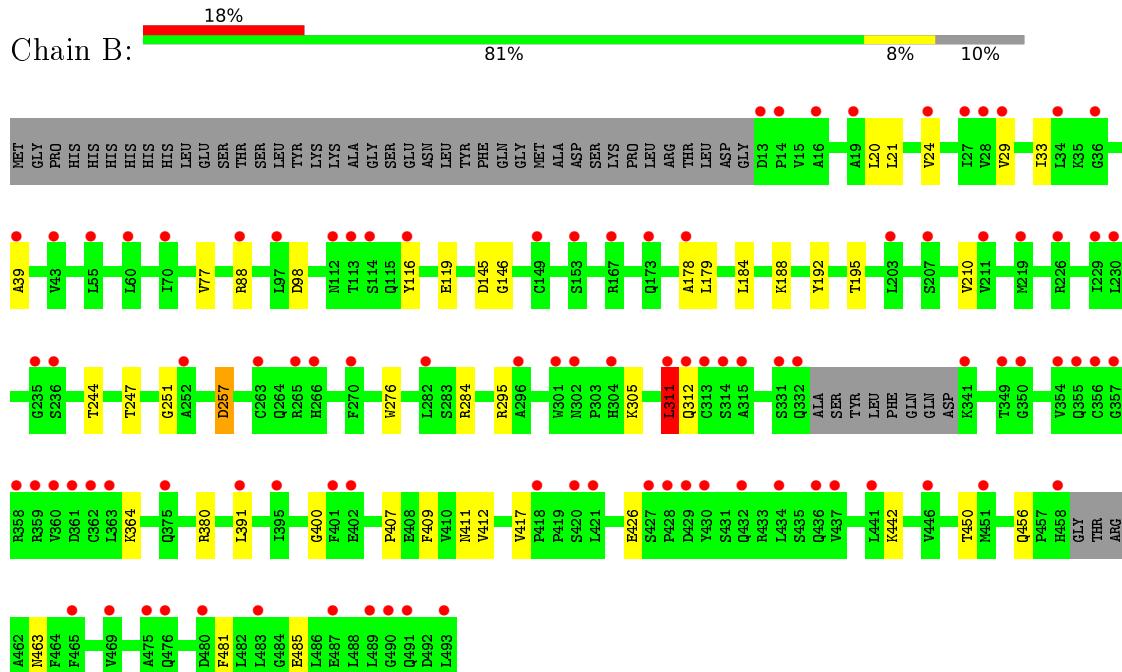
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

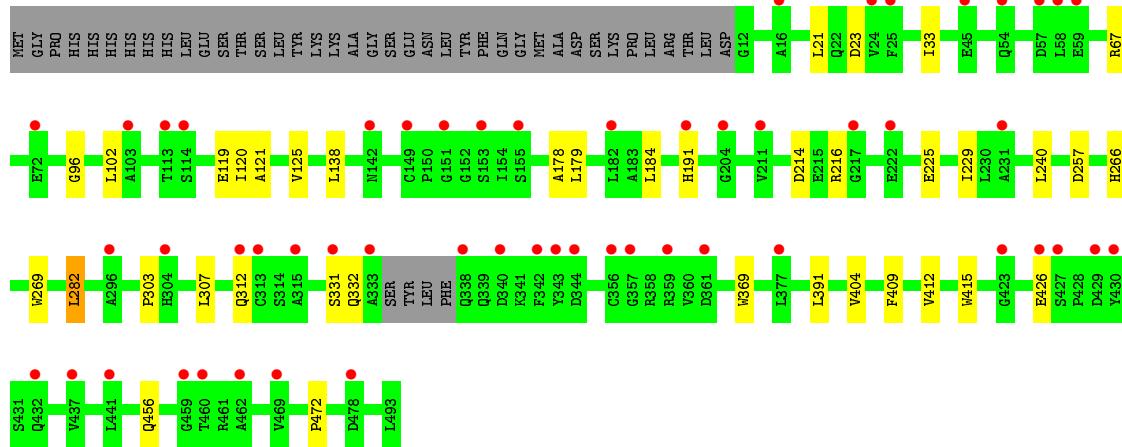
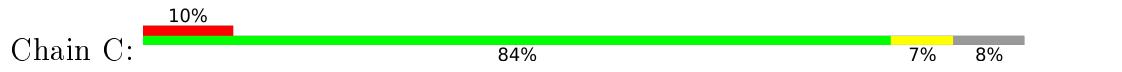
- Molecule 1: Cysteine sulfinic acid decarboxylase



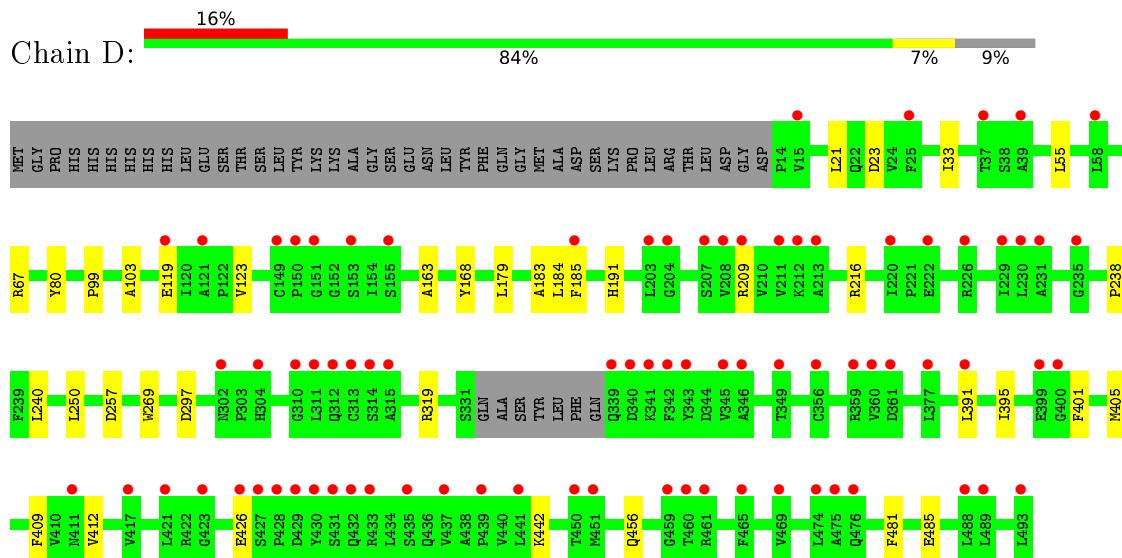
- Molecule 1: Cysteine sulfinic acid decarboxylase



- Molecule 1: Cysteine sulfenic acid decarboxylase



- Molecule 1: Cysteine sulfenic acid decarboxylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.06 Å 114.88 Å 113.76 Å 90.00° 95.80° 90.00°	Depositor
Resolution (Å)	47.02 – 2.80 47.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.02-2.80) 79.1 (47.02-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.43	Depositor
$< I/\sigma(I) >$ ¹	0.42 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.18rc7_3834	Depositor
R , R_{free}	0.243 , 0.292 0.243 , 0.291	Depositor DCC
R_{free} test set	2000 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 58.0	EDS
L-test for twinning ²	$< L > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	29915	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.27	0/3811	0.46	0/5149
1	B	0.27	0/3774	0.47	0/5100
1	C	0.28	0/3832	0.46	0/5179
1	D	0.27	0/3797	0.45	0/5131
All	All	0.28	0/15214	0.46	0/20559

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	311	LEU	Peptide

5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3736	3750	3748	17	0
1	B	3699	3716	3715	26	0
1	C	3756	3768	3767	24	0
1	D	3721	3741	3740	24	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	9	0	0	0	0
4	D	2	0	0	0	0
All	All	14940	14975	14970	75	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 3.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ASP:OD1	1:D:319:ARG:NH2	2.05	0.88
1:B:88:ARG:HD3	1:B:450:THR:O	1.79	0.82
1:C:225:GLU:OE1	1:C:266:HIS:NE2	2.13	0.82
1:B:39:ALA:O	1:B:88:ARG:NH2	2.20	0.74
1:B:21:LEU:HD13	1:D:33:ILE:HD13	1.76	0.67
1:B:20:LEU:HD23	1:D:99:PRO:HB2	1.76	0.67
1:B:21:LEU:CD1	1:D:33:ILE:HD13	2.30	0.62
1:C:225:GLU:OE2	1:C:229:ILE:HG13	1.99	0.61
1:B:98:ASP:OD2	1:B:380:ARG:NH1	2.33	0.60
1:B:311:LEU:O	1:B:364:LYS:NZ	2.21	0.60
1:C:225:GLU:CD	1:C:266:HIS:NE2	2.57	0.57
1:B:391:LEU:HD23	1:B:412:VAL:HG21	1.86	0.57
1:B:400:GLY:O	1:B:417:VAL:N	2.35	0.56
1:D:55:LEU:HD11	1:D:80:TYR:CZ	2.40	0.56
1:C:23:ASP:OD2	1:C:67:ARG:NH2	2.40	0.55
1:D:55:LEU:O	1:D:55:LEU:HD23	2.05	0.55
1:B:276:TRP:HE1	1:B:411:ASN:HD21	1.54	0.55
1:A:442:LYS:NZ	1:C:119:GLU:OE2	2.35	0.55
1:A:33:ILE:HD13	1:C:21:LEU:CD1	2.37	0.55
1:C:33:ILE:HD11	1:C:102:LEU:HD21	1.89	0.54
1:C:404:VAL:HG22	1:C:415:TRP:CZ3	2.42	0.54
1:A:55:LEU:HD11	1:A:80:TYR:OH	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:GLU:OE2	1:C:266:HIS:CE1	2.61	0.54
1:D:23:ASP:OD2	1:D:67:ARG:NH2	2.41	0.54
1:B:442:LYS:NZ	1:D:119:GLU:OE2	2.36	0.52
1:C:225:GLU:OE2	1:C:229:ILE:CG1	2.58	0.52
1:A:97:LEU:O	1:A:97:LEU:HD23	2.09	0.52
1:B:29:VAL:HA	1:B:33:ILE:HD12	1.92	0.51
1:D:55:LEU:HD11	1:D:80:TYR:OH	2.11	0.50
1:A:33:ILE:HD13	1:C:21:LEU:HD13	1.94	0.49
1:B:257:ASP:OD1	1:B:295:ARG:NH1	2.39	0.49
1:D:240:LEU:HD12	1:D:269:TRP:CD1	2.47	0.49
1:A:171:CYS:HB2	1:A:179:LEU:HD21	1.95	0.49
1:B:119:GLU:OE2	1:D:442:LYS:NZ	2.44	0.48
1:B:33:ILE:HD13	1:D:21:LEU:CD1	2.44	0.48
1:D:250:LEU:HD22	1:D:405:MET:SD	2.53	0.48
1:B:251:GLY:HA3	1:B:411:ASN:HD22	1.78	0.48
1:A:434:LEU:HD23	1:A:461:ARG:NH1	2.29	0.47
1:B:33:ILE:HD13	1:D:21:LEU:HD13	1.96	0.47
1:D:481:PHE:O	1:D:485:GLU:N	2.42	0.45
1:C:121:ALA:O	1:C:125:VAL:HG23	2.16	0.45
1:C:303:PRO:HB3	1:C:307:LEU:HD12	1.99	0.45
1:A:357:GLY:O	1:C:312:GLN:NE2	2.49	0.45
1:D:185:PHE:CD2	1:D:209:ARG:HB2	2.52	0.45
1:B:244:THR:HG21	1:B:247:THR:HG22	1.99	0.44
1:C:240:LEU:HD12	1:C:269:TRP:CD1	2.53	0.44
1:A:192:TYR:CE2	1:C:331:SER:HB2	2.53	0.44
1:A:481:PHE:O	1:A:485:GLU:N	2.40	0.43
1:D:395:ILE:HG23	1:D:401:PHE:HB3	1.99	0.43
1:A:387:LEU:HD13	1:A:474:LEU:HB3	2.00	0.43
1:D:391:LEU:HD23	1:D:412:VAL:HG21	2.00	0.43
1:B:188:LYS:HD3	1:B:210:VAL:HG11	2.01	0.42
1:B:145:ASP:OD1	1:B:146:GLY:N	2.49	0.42
1:C:214:ASP:OD1	1:C:216:ARG:N	2.52	0.42
1:B:481:PHE:O	1:B:485:GLU:N	2.44	0.42
1:C:96:GLY:HA3	1:C:472:PRO:HD2	2.02	0.42
1:B:178:ALA:C	1:B:179:LEU:HD12	2.40	0.42
1:B:276:TRP:CZ3	1:B:305:LYS:HB3	2.55	0.42
1:A:147:VAL:HG22	1:A:148:PHE:N	2.34	0.42
1:C:178:ALA:C	1:C:179:LEU:HD12	2.41	0.42
1:D:168:TYR:HB2	1:D:179:LEU:HD21	2.02	0.42
1:A:60:LEU:HD13	1:C:369:TRP:CD2	2.56	0.41
1:C:138:LEU:HD13	1:C:282:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:HD23	1:C:412:VAL:HG21	2.02	0.41
1:A:434:LEU:HD23	1:A:461:ARG:HH12	1.86	0.41
1:B:24:VAL:HG11	1:D:103:ALA:HB1	2.02	0.41
1:A:23:ASP:OD2	1:A:67:ARG:NH2	2.54	0.41
1:B:77:VAL:HG13	1:D:123:VAL:HG11	2.02	0.41
1:D:216:ARG:HD3	1:D:405:MET:HE3	2.03	0.41
1:A:82:VAL:HG21	1:C:120:ILE:HA	2.02	0.41
1:C:225:GLU:OE2	1:C:266:HIS:NE2	2.54	0.41
1:A:188:LYS:O	1:A:188:LYS:HE3	2.21	0.40
1:B:407:PRO:HB3	1:B:411:ASN:O	2.20	0.40
1:D:163:ALA:HB2	1:D:269:TRP:CG	2.56	0.40
1:D:183:ALA:O	1:D:238:PRO:HA	2.21	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	468/521 (90%)	448 (96%)	20 (4%)	0	100 100
1	B	464/521 (89%)	444 (96%)	17 (4%)	3 (1%)	25 56
1	C	474/521 (91%)	453 (96%)	21 (4%)	0	100 100
1	D	469/521 (90%)	448 (96%)	21 (4%)	0	100 100
All	All	1875/2084 (90%)	1793 (96%)	79 (4%)	3 (0%)	47 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	LEU
1	B	312	GLN
1	B	463	ASN

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	401/440 (91%)	393 (98%)	8 (2%)	55 84
1	B	397/440 (90%)	388 (98%)	9 (2%)	50 82
1	C	402/440 (91%)	394 (98%)	8 (2%)	55 84
1	D	399/440 (91%)	393 (98%)	6 (2%)	65 89
All	All	1599/1760 (91%)	1568 (98%)	31 (2%)	57 85

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	LEU
1	A	188	LYS
1	A	192	TYR
1	A	257	ASP
1	A	313	CYS
1	A	409	PHE
1	A	426	GLU
1	A	491	GLN
1	B	116	TYR
1	B	184	LEU
1	B	192	TYR
1	B	195	THR
1	B	257	ASP
1	B	284	ARG
1	B	409	PHE
1	B	426	GLU
1	B	456	GLN
1	C	184	LEU
1	C	191	HIS
1	C	257	ASP
1	C	282	LEU
1	C	332	GLN
1	C	409	PHE
1	C	426	GLU

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Mol	Chain	Res	Type
1	C	456	GLN
1	D	184	LEU
1	D	191	HIS
1	D	257	ASP
1	D	409	PHE
1	D	426	GLU
1	D	456	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	458	HIS
1	B	92	GLN
1	B	411	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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.10	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.

No monomer is involved in short contacts.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	474/521 (90%)	0.85	55 (11%) 4 2	37, 54, 73, 99	0
1	B	470/521 (90%)	1.20	96 (20%) 1 0	44, 64, 82, 94	0
1	C	478/521 (91%)	0.89	54 (11%) 5 3	39, 55, 76, 91	0
1	D	473/521 (90%)	1.16	81 (17%) 1 1	45, 64, 83, 101	0
All	All	1895/2084 (90%)	1.02	286 (15%) 2 1	37, 60, 79, 101	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	PRO	5.6
1	D	437	VAL	5.5
1	B	489	LEU	5.4
1	D	460	THR	5.3
1	B	437	VAL	5.2
1	B	235	GLY	4.8
1	D	400	GLY	4.8
1	B	421	LEU	4.8
1	A	432	GLN	4.7
1	B	357	GLY	4.6
1	D	229	ILE	4.6
1	B	432	GLN	4.6
1	D	493	LEU	4.5
1	D	428	PRO	4.5
1	B	475	ALA	4.5
1	B	356	CYS	4.5
1	D	339	GLN	4.5
1	D	432	GLN	4.4
1	D	211	VAL	4.4
1	C	58	LEU	4.3
1	D	340	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	460	THR	4.2
1	D	235	GLY	4.2
1	A	332	GLN	4.1
1	A	311	LEU	4.1
1	D	342	PHE	4.1
1	D	341	LYS	4.1
1	B	359	ARG	4.1
1	B	429	ASP	4.1
1	B	312	GLN	4.0
1	B	24	VAL	4.0
1	D	39	ALA	4.0
1	C	427	SER	3.9
1	C	356	CYS	3.9
1	D	312	GLN	3.9
1	A	313	CYS	3.8
1	B	491	GLN	3.8
1	B	16	ALA	3.8
1	B	265	ARG	3.7
1	A	54	GLN	3.7
1	B	311	LEU	3.6
1	C	426	GLU	3.5
1	C	423	GLY	3.5
1	D	231	ALA	3.5
1	D	311	LEU	3.5
1	A	339	GLN	3.5
1	A	338	GLN	3.4
1	D	151	GLY	3.4
1	D	450	THR	3.4
1	C	361	ASP	3.4
1	B	493	LEU	3.4
1	A	461	ARG	3.3
1	D	230	LEU	3.3
1	D	429	ASP	3.3
1	A	153	SER	3.3
1	D	313	CYS	3.3
1	C	331	SER	3.3
1	A	435	SER	3.3
1	A	312	GLN	3.3
1	C	340	ASP	3.3
1	D	304	HIS	3.3
1	D	459	GLY	3.3
1	C	114	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	173	GLN	3.2
1	B	362	CYS	3.2
1	C	342	PHE	3.2
1	D	121	ALA	3.2
1	D	213	ALA	3.2
1	A	15	VAL	3.2
1	B	360	VAL	3.2
1	B	39	ALA	3.2
1	B	270	PHE	3.1
1	C	142	ASN	3.1
1	A	469	VAL	3.1
1	B	446	VAL	3.1
1	D	222	GLU	3.1
1	D	391	LEU	3.1
1	D	58	LEU	3.1
1	D	207	SER	3.1
1	C	333	ALA	3.0
1	D	310	GLY	3.0
1	B	114	SER	3.0
1	B	149	CYS	3.0
1	C	211	VAL	3.0
1	A	314	SER	3.0
1	A	302	ASN	3.0
1	B	302	ASN	3.0
1	B	313	CYS	3.0
1	C	313	CYS	3.0
1	D	361	ASP	3.0
1	B	418	PRO	2.9
1	C	357	GLY	2.9
1	A	426	GLU	2.9
1	D	423	GLY	2.9
1	A	304	HIS	2.9
1	A	67	ARG	2.9
1	D	417	VAL	2.9
1	D	343	TYR	2.9
1	B	207	SER	2.9
1	B	263	CYS	2.9
1	A	296	ALA	2.9
1	C	430	TYR	2.9
1	D	399	GLU	2.9
1	C	231	ALA	2.9
1	D	314	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	469	VAL	2.8
1	D	155	SER	2.8
1	D	37	THR	2.8
1	D	302	ASN	2.8
1	B	296	ALA	2.8
1	D	203	LEU	2.8
1	A	222	GLU	2.7
1	B	402	GLU	2.7
1	A	20	LEU	2.7
1	D	360	VAL	2.7
1	B	476	GLN	2.7
1	C	312	GLN	2.7
1	A	399	GLU	2.7
1	D	431	SER	2.7
1	B	361	ASP	2.7
1	B	427	SER	2.7
1	D	15	VAL	2.7
1	D	377	LEU	2.7
1	D	153	SER	2.7
1	D	430	TYR	2.7
1	C	338	GLN	2.6
1	A	13	ASP	2.6
1	D	209	ARG	2.6
1	D	475	ALA	2.6
1	B	341	LYS	2.6
1	B	332	GLN	2.6
1	C	182	LEU	2.6
1	B	282	LEU	2.6
1	C	469	VAL	2.6
1	D	150	PRO	2.6
1	B	314	SER	2.6
1	B	436	GLN	2.6
1	B	358	ARG	2.6
1	A	350	GLY	2.6
1	C	462	ALA	2.6
1	D	433	ARG	2.6
1	A	116	TYR	2.6
1	A	463	ASN	2.6
1	C	149	CYS	2.6
1	D	226	ARG	2.6
1	C	54	GLN	2.6
1	D	451	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	211	VAL	2.6
1	C	432	GLN	2.5
1	B	113	THR	2.5
1	C	429	ASP	2.5
1	D	465	PHE	2.5
1	B	60	LEU	2.5
1	C	304	HIS	2.5
1	A	207	SER	2.5
1	B	395	ILE	2.5
1	B	430	TYR	2.5
1	C	441	LEU	2.5
1	B	458	HIS	2.5
1	C	72	GLU	2.5
1	B	252	ALA	2.5
1	A	421	LEU	2.5
1	C	217	GLY	2.5
1	B	153	SER	2.5
1	B	391	LEU	2.5
1	D	489	LEU	2.5
1	A	458	HIS	2.5
1	D	204	GLY	2.5
1	B	97	LEU	2.5
1	C	113	THR	2.4
1	D	474	LEU	2.4
1	C	155	SER	2.4
1	A	437	VAL	2.4
1	A	229	ILE	2.4
1	B	434	LEU	2.4
1	B	14	PRO	2.4
1	C	25	PHE	2.4
1	D	426	GLU	2.4
1	A	489	LEU	2.4
1	D	25	PHE	2.4
1	A	149	CYS	2.4
1	A	235	GLY	2.4
1	A	310	GLY	2.4
1	C	344	ASP	2.4
1	A	361	ASP	2.4
1	D	212	LYS	2.4
1	B	28	VAL	2.4
1	C	437	VAL	2.4
1	B	13	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	451	MET	2.4
1	A	356	CYS	2.3
1	A	209	ARG	2.3
1	B	19	ALA	2.3
1	B	230	LEU	2.3
1	C	153	SER	2.3
1	A	152	GLY	2.3
1	D	149	CYS	2.3
1	B	116	TYR	2.3
1	C	45	GLU	2.3
1	D	315	ALA	2.3
1	B	469	VAL	2.3
1	D	439	PRO	2.3
1	B	236	SER	2.3
1	B	483	LEU	2.3
1	A	151	GLY	2.3
1	D	461	ARG	2.3
1	B	36	GLY	2.3
1	D	345	VAL	2.2
1	C	204	GLY	2.2
1	A	430	TYR	2.2
1	A	226	ARG	2.2
1	C	24	VAL	2.2
1	A	142	ASN	2.2
1	B	112	ASN	2.2
1	D	427	SER	2.2
1	B	441	LEU	2.2
1	B	401	PHE	2.2
1	D	208	VAL	2.2
1	A	95	SER	2.2
1	C	151	GLY	2.2
1	B	487	GLU	2.2
1	D	441	LEU	2.2
1	B	34	LEU	2.2
1	A	94	PHE	2.2
1	B	226	ARG	2.2
1	C	359	ARG	2.2
1	D	349	THR	2.2
1	C	103	ALA	2.2
1	D	488	LEU	2.2
1	D	220	ILE	2.2
1	B	331	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	435	SER	2.2
1	A	113	THR	2.2
1	A	55	LEU	2.1
1	B	355	GLN	2.1
1	C	16	ALA	2.1
1	A	303	PRO	2.1
1	B	349	THR	2.1
1	C	57	ASP	2.1
1	C	377	LEU	2.1
1	B	354	VAL	2.1
1	D	356	CYS	2.1
1	D	476	GLN	2.1
1	B	219	MET	2.1
1	B	167	ARG	2.1
1	C	478	ASP	2.1
1	B	229	ILE	2.1
1	B	490	GLY	2.1
1	B	266	HIS	2.1
1	B	203	LEU	2.1
1	B	27	ILE	2.1
1	B	70	ILE	2.1
1	B	88	ARG	2.1
1	B	304	HIS	2.1
1	A	308	ALA	2.1
1	B	315	ALA	2.1
1	C	296	ALA	2.1
1	D	346	ALA	2.1
1	C	459	GLY	2.1
1	D	411	ASN	2.1
1	B	301	TRP	2.1
1	C	59	GLU	2.1
1	B	480	ASP	2.1
1	C	222	GLU	2.1
1	B	55	LEU	2.1
1	D	421	LEU	2.1
1	A	454	GLY	2.1
1	C	191	HIS	2.0
1	B	420	SER	2.0
1	B	178	ALA	2.0
1	B	350	GLY	2.0
1	B	29	VAL	2.0
1	B	465	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	441	LEU	2.0
1	D	185	PHE	2.0
1	A	359	ARG	2.0
1	B	375	GLN	2.0
1	D	359	ARG	2.0
1	C	343	TYR	2.0
1	A	345	VAL	2.0
1	B	43	VAL	2.0
1	A	355	GLN	2.0
1	A	400	GLY	2.0
1	D	119	GLU	2.0
1	C	315	ALA	2.0
1	B	363	LEU	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 monosaccharides 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
3	NA	C	501	1/1	0.79	0.26	50,50,50,50	0
2	SO4	A	501	5/5	0.84	0.47	65,75,88,99	0
3	NA	D	501	1/1	0.88	0.35	55,55,55,55	0
3	NA	A	502	1/1	0.91	0.09	27,27,27,27	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.