



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:51 AM UTC

PDB ID : 3S81 / pdb_00003s81
Title : Crystal Structure of Putative Aspartate Racemase from Salmonella Typhimurium
Authors : Maltseva, N.; Kim, Y.; Kwon, K.; Zhang, R.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-05-27
Resolution : 1.80 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

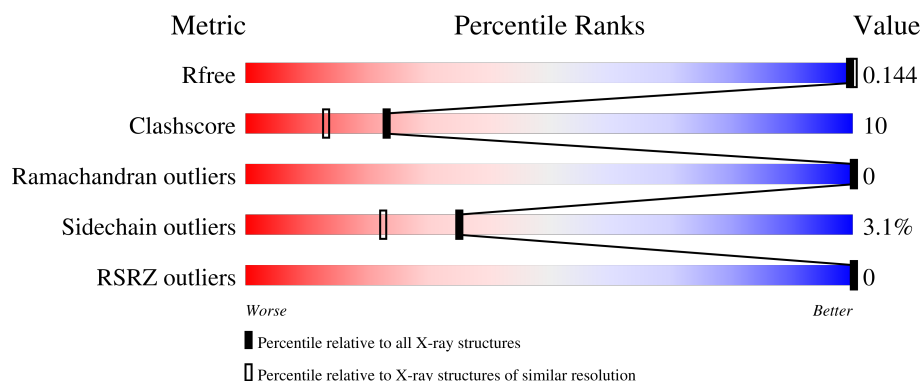
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	268	
1	B	268	
1	C	268	
1	D	268	

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	C	252	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7938 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 Putative aspartate racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	1	0
			1763	1117	307	325	14			
1	B	240	Total	C	N	O	S	0	3	0
			1848	1171	321	342	14			
1	C	239	Total	C	N	O	S	0	1	0
			1824	1157	318	335	14			
1	D	233	Total	C	N	O	S	0	2	0
			1787	1130	317	326	14			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q8ZJZ9
A	-22	HIS	-	expression tag	UNP Q8ZJZ9
A	-21	HIS	-	expression tag	UNP Q8ZJZ9
A	-20	HIS	-	expression tag	UNP Q8ZJZ9
A	-19	HIS	-	expression tag	UNP Q8ZJZ9
A	-18	HIS	-	expression tag	UNP Q8ZJZ9
A	-17	HIS	-	expression tag	UNP Q8ZJZ9
A	-16	SER	-	expression tag	UNP Q8ZJZ9
A	-15	SER	-	expression tag	UNP Q8ZJZ9
A	-14	GLY	-	expression tag	UNP Q8ZJZ9
A	-13	VAL	-	expression tag	UNP Q8ZJZ9
A	-12	ASP	-	expression tag	UNP Q8ZJZ9
A	-11	LEU	-	expression tag	UNP Q8ZJZ9
A	-10	GLY	-	expression tag	UNP Q8ZJZ9
A	-9	THR	-	expression tag	UNP Q8ZJZ9
A	-8	GLU	-	expression tag	UNP Q8ZJZ9
A	-7	ASN	-	expression tag	UNP Q8ZJZ9
A	-6	LEU	-	expression tag	UNP Q8ZJZ9
A	-5	TYR	-	expression tag	UNP Q8ZJZ9
A	-4	PHE	-	expression tag	UNP Q8ZJZ9
A	-3	GLN	-	expression tag	UNP Q8ZJZ9

Continued on next page...

Continued from previous page...

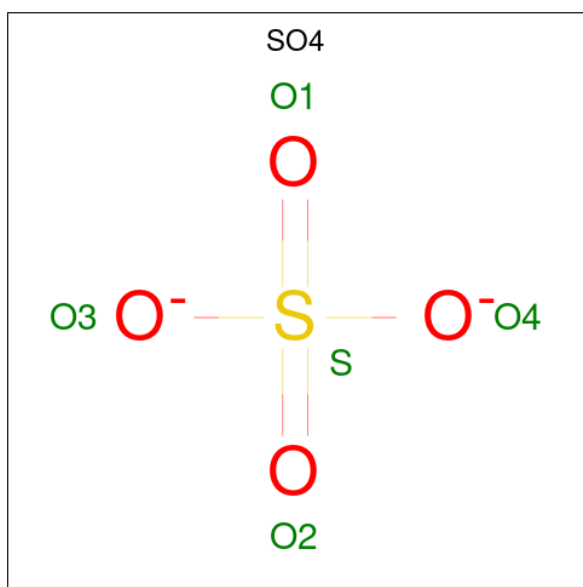
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8ZJZ9
A	-1	ASN	-	expression tag	UNP Q8ZJZ9
A	0	ALA	-	expression tag	UNP Q8ZJZ9
B	-23	MET	-	expression tag	UNP Q8ZJZ9
B	-22	HIS	-	expression tag	UNP Q8ZJZ9
B	-21	HIS	-	expression tag	UNP Q8ZJZ9
B	-20	HIS	-	expression tag	UNP Q8ZJZ9
B	-19	HIS	-	expression tag	UNP Q8ZJZ9
B	-18	HIS	-	expression tag	UNP Q8ZJZ9
B	-17	HIS	-	expression tag	UNP Q8ZJZ9
B	-16	SER	-	expression tag	UNP Q8ZJZ9
B	-15	SER	-	expression tag	UNP Q8ZJZ9
B	-14	GLY	-	expression tag	UNP Q8ZJZ9
B	-13	VAL	-	expression tag	UNP Q8ZJZ9
B	-12	ASP	-	expression tag	UNP Q8ZJZ9
B	-11	LEU	-	expression tag	UNP Q8ZJZ9
B	-10	GLY	-	expression tag	UNP Q8ZJZ9
B	-9	THR	-	expression tag	UNP Q8ZJZ9
B	-8	GLU	-	expression tag	UNP Q8ZJZ9
B	-7	ASN	-	expression tag	UNP Q8ZJZ9
B	-6	LEU	-	expression tag	UNP Q8ZJZ9
B	-5	TYR	-	expression tag	UNP Q8ZJZ9
B	-4	PHE	-	expression tag	UNP Q8ZJZ9
B	-3	GLN	-	expression tag	UNP Q8ZJZ9
B	-2	SER	-	expression tag	UNP Q8ZJZ9
B	-1	ASN	-	expression tag	UNP Q8ZJZ9
B	0	ALA	-	expression tag	UNP Q8ZJZ9
C	-23	MET	-	expression tag	UNP Q8ZJZ9
C	-22	HIS	-	expression tag	UNP Q8ZJZ9
C	-21	HIS	-	expression tag	UNP Q8ZJZ9
C	-20	HIS	-	expression tag	UNP Q8ZJZ9
C	-19	HIS	-	expression tag	UNP Q8ZJZ9
C	-18	HIS	-	expression tag	UNP Q8ZJZ9
C	-17	HIS	-	expression tag	UNP Q8ZJZ9
C	-16	SER	-	expression tag	UNP Q8ZJZ9
C	-15	SER	-	expression tag	UNP Q8ZJZ9
C	-14	GLY	-	expression tag	UNP Q8ZJZ9
C	-13	VAL	-	expression tag	UNP Q8ZJZ9
C	-12	ASP	-	expression tag	UNP Q8ZJZ9
C	-11	LEU	-	expression tag	UNP Q8ZJZ9
C	-10	GLY	-	expression tag	UNP Q8ZJZ9
C	-9	THR	-	expression tag	UNP Q8ZJZ9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q8ZJZ9
C	-7	ASN	-	expression tag	UNP Q8ZJZ9
C	-6	LEU	-	expression tag	UNP Q8ZJZ9
C	-5	TYR	-	expression tag	UNP Q8ZJZ9
C	-4	PHE	-	expression tag	UNP Q8ZJZ9
C	-3	GLN	-	expression tag	UNP Q8ZJZ9
C	-2	SER	-	expression tag	UNP Q8ZJZ9
C	-1	ASN	-	expression tag	UNP Q8ZJZ9
C	0	ALA	-	expression tag	UNP Q8ZJZ9
D	-23	MET	-	expression tag	UNP Q8ZJZ9
D	-22	HIS	-	expression tag	UNP Q8ZJZ9
D	-21	HIS	-	expression tag	UNP Q8ZJZ9
D	-20	HIS	-	expression tag	UNP Q8ZJZ9
D	-19	HIS	-	expression tag	UNP Q8ZJZ9
D	-18	HIS	-	expression tag	UNP Q8ZJZ9
D	-17	HIS	-	expression tag	UNP Q8ZJZ9
D	-16	SER	-	expression tag	UNP Q8ZJZ9
D	-15	SER	-	expression tag	UNP Q8ZJZ9
D	-14	GLY	-	expression tag	UNP Q8ZJZ9
D	-13	VAL	-	expression tag	UNP Q8ZJZ9
D	-12	ASP	-	expression tag	UNP Q8ZJZ9
D	-11	LEU	-	expression tag	UNP Q8ZJZ9
D	-10	GLY	-	expression tag	UNP Q8ZJZ9
D	-9	THR	-	expression tag	UNP Q8ZJZ9
D	-8	GLU	-	expression tag	UNP Q8ZJZ9
D	-7	ASN	-	expression tag	UNP Q8ZJZ9
D	-6	LEU	-	expression tag	UNP Q8ZJZ9
D	-5	TYR	-	expression tag	UNP Q8ZJZ9
D	-4	PHE	-	expression tag	UNP Q8ZJZ9
D	-3	GLN	-	expression tag	UNP Q8ZJZ9
D	-2	SER	-	expression tag	UNP Q8ZJZ9
D	-1	ASN	-	expression tag	UNP Q8ZJZ9
D	0	ALA	-	expression tag	UNP Q8ZJZ9

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



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

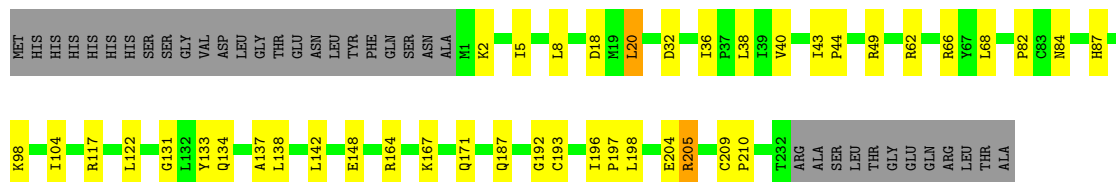
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	166	Total	O	0	0
			166	166		
4	B	161	Total	O	0	0
			161	161		
4	C	176	Total	O	0	0
			176	176		
4	D	158	Total	O	0	0
			158	158		

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.

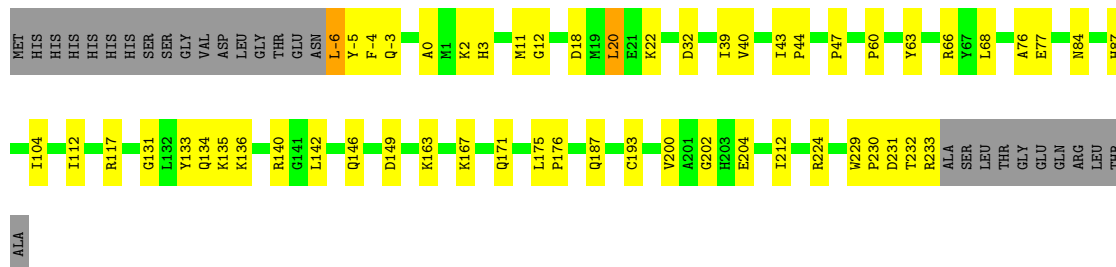
• Molecule 1: Putative aspartate racemase

Chain A: 



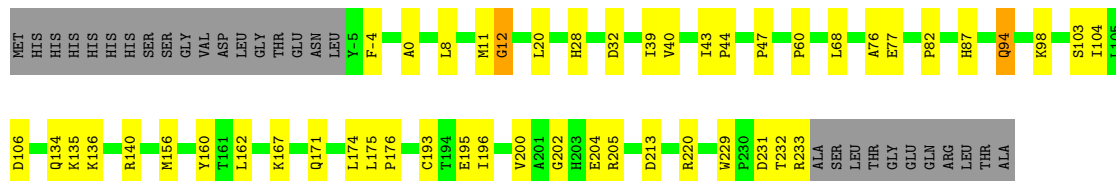
• Molecule 1: Putative aspartate racemase

Chain B: 



• Molecule 1: Putative aspartate racemase

Chain C: 



• Molecule 1: Putative aspartate racemase

Chain D: 

MET	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	VAL	ASP	LEU	GLY	THR	GLU	ASN	LEU	TYR	PHE	GLN	SER	ASN	ALA	M1	I5	L8	G12	L20	H28	D32	I36	V40	I43	P44	S55	R62	R66	E77	P82	C83	N84	H87	V96
I104	L122	M125	Y133	Q134	K135	L138	L144	E148	M156	Y160	R164	G165	D166	K167	Q171	L175	M191	G192	C193	I196	V200	H203	E204	R205	R224	W229	T232	R233	ALA	SER	LEU	THR	GLY	GLU	GLN	ARG	LEU	THR	ALA			

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	84.15Å 84.15Å 114.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.04 – 1.80 45.04 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.04-1.80) 99.8 (45.04-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.140 , 0.169 0.136 , 0.144	Depositor DCC
R_{free} test set	4216 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.447 for -h,-k,l 0.205 for h,-h-k,-l 0.198 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7938	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: CL, 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	0.49	0/1798	0.92	2/2448 (0.1%)
1	B	0.49	0/1885	0.89	2/2566 (0.1%)
1	C	0.48	0/1861	0.90	4/2533 (0.2%)
1	D	0.49	0/1822	0.94	7/2478 (0.3%)
All	All	0.49	0/7366	0.91	15/10025 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	ILE	CA-C-N	11.03	131.34	119.87
1	D	43	ILE	C-N-CA	11.03	131.34	119.87
1	B	43	ILE	CA-C-N	10.29	130.57	119.87
1	B	43	ILE	C-N-CA	10.29	130.57	119.87
1	A	43	ILE	CA-C-N	10.01	130.28	119.87
1	A	43	ILE	C-N-CA	10.01	130.28	119.87
1	C	43	ILE	CA-C-N	9.81	130.07	119.87
1	C	43	ILE	C-N-CA	9.81	130.07	119.87
1	D	12	GLY	CA-C-N	6.89	126.70	119.05
1	D	12	GLY	C-N-CA	6.89	126.70	119.05
1	C	12	GLY	CA-C-N	5.88	125.58	119.05
1	C	12	GLY	C-N-CA	5.88	125.58	119.05
1	D	55	SER	N-CA-C	5.17	119.28	112.92
1	D	165	GLY	N-CA-C	5.16	121.87	114.64
1	D	203	HIS	N-CA-C	5.12	119.62	113.17

There are no chirality outliers.

There are no planarity outliers.

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	1763	0	1796	33	0
1	B	1848	0	1871	63	0
1	C	1824	0	1854	37	0
1	D	1787	0	1826	47	0
2	A	10	0	0	0	0
2	B	15	0	0	2	0
2	C	15	0	0	2	0
2	D	10	0	0	0	0
3	A	2	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
4	A	166	0	0	3	0
4	B	161	0	0	7	0
4	C	176	0	0	5	0
4	D	158	0	0	5	0
All	All	7938	0	7347	151	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 10.

All (151) 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:233:ARG:HG3	1:D:233:ARG:HH11	1.22	1.02
1:D:232:THR:O	1:D:233:ARG:HB2	1.64	0.97
1:B:-6:LEU:HD12	1:B:-5:TYR:H	1.31	0.96
1:D:233:ARG:HH11	1:D:233:ARG:CG	1.90	0.85
1:D:233:ARG:HG3	1:D:233:ARG:NH1	1.88	0.78
1:B:224:ARG:HE	1:D:233:ARG:HD3	1.49	0.77
1:B:233:ARG:HD2	1:D:224:ARG:HH21	1.57	0.70
1:A:205:ARG:HH21	1:A:205:ARG:HG2	1.57	0.69
1:B:193:CYS:HA	3:B:251:CL:CL	2.33	0.66
1:A:205:ARG:HG2	1:A:205:ARG:NH2	2.11	0.66
1:C:-4:PHE:HB3	1:D:66:ARG:NH1	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:TYR:O	1:D:164[B]:ARG:HG3	1.96	0.65
1:A:20:LEU:HD11	1:A:40:VAL:HG21	1.78	0.65
1:C:167:LYS:HE2	1:C:171:GLN:NE2	2.12	0.64
1:A:117:ARG:NH2	4:A:475:HOH:O	2.31	0.63
1:A:66:ARG:NH1	1:B:-4:PHE:HB3	2.14	0.63
1:D:138:LEU:HD13	4:D:476:HOH:O	1.99	0.63
1:B:200:VAL:HG12	1:B:204:GLU:HG3	1.81	0.61
1:B:39[B]:ILE:HD11	1:B:76:ALA:HB2	1.81	0.61
1:D:171:GLN:O	1:D:175:LEU:HG	2.00	0.61
1:A:167:LYS:O	1:A:171:GLN:HG3	2.01	0.60
1:B:-3:GLN:HB3	1:B:2:LYS:HE3	1.84	0.60
1:D:125:ASN:ND2	1:D:156:MET:HG3	2.17	0.59
1:C:193:CYS:HA	3:C:251:CL:CL	2.40	0.58
1:D:191:MET:SD	1:D:200:VAL:HG11	2.44	0.58
1:D:28:HIS:ND1	4:D:279:HOH:O	2.32	0.58
1:B:224:ARG:HE	1:D:233:ARG:CD	2.16	0.57
1:D:196:ILE:O	1:D:200:VAL:HG12	2.05	0.57
1:C:205:ARG:HG3	2:C:252:SO4:O4	2.04	0.57
1:D:167:LYS:O	1:D:171:GLN:HG3	2.05	0.56
1:C:232:THR:O	1:C:233:ARG:HB2	2.04	0.56
1:A:40:VAL:HB	1:B:40:VAL:HB	1.88	0.56
1:C:156:MET:HE3	1:C:160:TYR:CE1	2.41	0.55
1:D:232:THR:O	1:D:233:ARG:CB	2.48	0.55
1:B:233:ARG:CD	1:D:224:ARG:HH21	2.19	0.55
2:B:253:SO4:O3	4:B:657:HOH:O	2.17	0.55
1:C:44:PRO:HB2	1:D:32:ASP:O	2.06	0.55
1:A:66:ARG:CZ	1:B:-4:PHE:HB2	2.37	0.55
1:A:193:CYS:HB3	1:A:196:ILE:HG12	1.89	0.54
1:A:193:CYS:HA	3:A:251:CL:CL	2.44	0.54
1:B:224:ARG:HE	1:D:233:ARG:HG2	1.72	0.54
1:D:193:CYS:HA	3:D:251:CL:CL	2.44	0.54
1:C:39[B]:ILE:HD11	1:C:76:ALA:HB2	1.90	0.54
1:A:32:ASP:O	1:B:44:PRO:HB2	2.08	0.54
1:C:-4:PHE:HB2	1:D:66:ARG:CZ	2.38	0.54
1:A:44:PRO:HB2	1:B:32:ASP:O	2.08	0.53
1:B:18:ASP:OD2	1:B:22:LYS:HE2	2.09	0.53
1:A:5:ILE:HD12	1:A:36:ILE:HG21	1.90	0.53
1:D:135:LYS:HB2	4:D:484:HOH:O	2.08	0.53
1:C:202:GLY:N	2:C:252:SO4:O2	2.41	0.53
1:D:87:HIS:CE1	1:D:104:ILE:HG22	2.43	0.53
1:A:62:ARG:HB2	4:A:487:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:HH21	1:A:205:ARG:CG	2.21	0.53
1:B:171:GLN:O	1:B:175:LEU:HG	2.09	0.52
1:B:233:ARG:HB2	1:D:224:ARG:HE	1.74	0.52
1:D:193:CYS:HB3	1:D:196:ILE:HG12	1.90	0.52
1:B:3:HIS:ND1	4:B:561:HOH:O	2.33	0.52
1:C:94:GLN:HE21	1:C:94:GLN:HA	1.75	0.52
1:C:229:TRP:HB2	1:C:232:THR:OG1	2.09	0.52
1:B:-6:LEU:CD1	1:B:-5:TYR:H	2.11	0.52
1:C:32:ASP:O	1:D:44:PRO:HB2	2.08	0.52
1:B:229:TRP:HB2	1:B:232:THR:OG1	2.11	0.51
1:B:47:PRO:HD2	1:B:60:PRO:HA	1.92	0.51
1:A:20:LEU:HD22	1:B:20:LEU:HD12	1.91	0.51
1:C:-4:PHE:CB	1:D:66:ARG:NH1	2.73	0.51
1:C:136:LYS:HG3	4:C:497:HOH:O	2.11	0.51
1:B:232:THR:O	1:B:233:ARG:CB	2.58	0.50
1:B:-4:PHE:O	1:B:-4:PHE:HD1	1.95	0.50
3:A:253:CL:CL	1:B:163:LYS:HD3	2.48	0.50
1:A:66:ARG:NH1	1:B:-4:PHE:CB	2.75	0.49
1:B:224:ARG:NE	1:D:233:ARG:HD3	2.25	0.49
1:A:18:ASP:HB2	1:A:198:LEU:HD21	1.95	0.49
1:B:224:ARG:HE	1:D:233:ARG:CG	2.25	0.49
1:B:135:LYS:HB3	4:B:324:HOH:O	2.11	0.49
1:B:233:ARG:HH21	1:D:224:ARG:HH21	1.59	0.49
1:D:134:GLN:NE2	1:D:144:LEU:HD12	2.28	0.49
1:C:94:GLN:HE21	1:C:94:GLN:CA	2.25	0.49
1:B:140:ARG:NH2	4:B:314:HOH:O	2.41	0.48
1:C:47:PRO:HD2	1:C:60:PRO:HA	1.96	0.48
1:B:131:GLY:HA2	1:B:134:GLN:OE1	2.13	0.48
1:C:28:HIS:HA	4:C:442:HOH:O	2.13	0.48
1:B:232:THR:O	1:B:233:ARG:HB2	2.14	0.48
1:B:229:TRP:HE3	1:B:230:PRO:HD2	1.78	0.48
1:C:135:LYS:HG3	4:C:576:HOH:O	2.13	0.48
1:C:87:HIS:CE1	1:C:104:ILE:HG22	2.50	0.47
1:C:229:TRP:O	1:C:233:ARG:N	2.47	0.47
1:B:202:GLY:N	2:B:252:SO4:O1	2.47	0.47
1:B:233:ARG:HD2	1:D:224:ARG:NH2	2.27	0.46
1:B:200:VAL:HG12	1:B:204:GLU:CG	2.45	0.46
1:B:0:ALA:HA	1:B:77:GLU:HG2	1.97	0.46
1:A:122:LEU:O	1:A:192:GLY:N	2.47	0.46
1:B:63:TYR:CD1	1:B:66:ARG:NH1	2.85	0.45
1:B:224:ARG:CB	1:D:233:ARG:HG2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:VAL:HB	1:D:40:VAL:HB	1.98	0.45
1:D:229:TRP:O	1:D:233:ARG:N	2.50	0.45
1:B:-4:PHE:O	1:B:-4:PHE:CD1	2.69	0.45
1:D:8:LEU:O	1:D:82:PRO:HD2	2.16	0.45
1:B:175:LEU:N	1:B:176:PRO:CD	2.79	0.45
1:C:20:LEU:HD12	1:D:20:LEU:HD12	1.99	0.45
1:D:84:ASN:ND2	1:D:133:TYR:OH	2.49	0.45
1:D:122:LEU:HA	4:D:253:HOH:O	2.17	0.45
1:B:175:LEU:HB2	1:B:176:PRO:HD3	1.99	0.44
1:D:5:ILE:HD12	1:D:36:ILE:HG21	1.99	0.44
1:D:77:GLU:HG3	4:D:598:HOH:O	2.17	0.44
1:B:-3:GLN:O	4:B:328:HOH:O	2.21	0.44
1:C:8:LEU:O	1:C:82:PRO:HD2	2.18	0.44
1:A:49:ARG:N	1:A:49:ARG:HD3	2.33	0.44
1:B:136:LYS:HG3	4:B:324:HOH:O	2.18	0.44
1:A:8:LEU:O	1:A:82:PRO:HD2	2.18	0.43
1:B:-6:LEU:HD12	1:B:-5:TYR:N	2.15	0.43
1:B:117:ARG:N	1:B:187:GLN:OE1	2.49	0.43
1:B:233:ARG:HD2	1:D:224:ARG:HE	1.83	0.43
1:A:84:ASN:ND2	1:A:133:TYR:OH	2.51	0.43
1:A:209:CYS:HB2	1:A:210:PRO:HD2	2.00	0.43
1:B:84:ASN:ND2	1:B:133:TYR:OH	2.52	0.43
1:B:11:MET:HA	1:B:12:GLY:HA2	1.86	0.43
1:B:87:HIS:CE1	1:B:104:ILE:HG22	2.53	0.43
1:B:233:ARG:HH21	1:D:224:ARG:NH2	2.15	0.43
1:B:-3:GLN:O	1:B:2:LYS:HE3	2.19	0.43
1:B:112:ILE:HG12	1:B:212:ILE:HG13	2.01	0.43
1:A:66:ARG:HH11	1:B:-4:PHE:HB3	1.81	0.43
1:C:200:VAL:HG12	1:C:204:GLU:HG3	2.01	0.42
1:C:193:CYS:HB3	1:C:196:ILE:HG12	2.02	0.42
1:C:175:LEU:HB2	1:C:176:PRO:HD3	2.00	0.42
1:B:134:GLN:HE22	1:B:146:GLN:NE2	2.16	0.42
1:C:162:LEU:HD12	1:C:195:GLU:CG	2.49	0.42
1:C:174:LEU:HD21	1:C:196:ILE:HG23	1.99	0.42
1:A:117:ARG:N	1:A:187:GLN:OE1	2.53	0.42
1:C:0:ALA:HA	1:C:77:GLU:HG2	2.02	0.42
1:B:0:ALA:HB1	1:B:77:GLU:OE2	2.20	0.42
1:C:-4:PHE:CB	1:D:66:ARG:CZ	2.98	0.42
1:D:138:LEU:HD12	1:D:138:LEU:HA	1.90	0.42
1:C:140:ARG:NE	4:C:344:HOH:O	2.39	0.42
1:C:175:LEU:N	1:C:176:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:CE1	1:A:104:ILE:HG22	2.54	0.42
1:A:196:ILE:HB	1:A:197:PRO:HD3	2.02	0.42
1:B:167:LYS:O	1:B:171:GLN:HG3	2.20	0.42
1:B:149[B]:ASP:OD1	1:B:149[B]:ASP:C	2.62	0.41
1:A:164:ARG:NH1	4:A:285:HOH:O	2.53	0.41
1:A:137:ALA:HB1	1:A:142:LEU:HB2	2.01	0.41
1:B:142:LEU:HD21	4:B:309:HOH:O	2.20	0.41
1:B:232:THR:O	1:B:233:ARG:HG3	2.20	0.41
1:C:11:MET:HA	1:C:12:GLY:HA2	1.82	0.41
1:A:5:ILE:HB	1:A:38:LEU:HD23	2.01	0.41
1:A:193:CYS:HB3	1:A:196:ILE:CG1	2.50	0.41
1:A:66:ARG:CZ	1:B:-4:PHE:CB	3.00	0.40
1:C:103:SER:HB3	1:C:106:ASP:OD1	2.20	0.40
1:A:131:GLY:HA2	1:A:134[A]:GLN:HG2	2.02	0.40
1:C:213:ASP:OD1	1:C:213:ASP:C	2.64	0.40
1:C:220:ARG:NH2	4:C:274:HOH:O	2.51	0.40
1:D:193:CYS:HB3	1:D:196:ILE:CG1	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/268 (86%)	231 (100%)	0	0	100	100
1	B	241/268 (90%)	240 (100%)	1 (0%)	0	100	100
1	C	238/268 (89%)	238 (100%)	0	0	100	100
1	D	233/268 (87%)	233 (100%)	0	0	100	100
All	All	943/1072 (88%)	942 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	185/214 (86%)	177 (96%)	8 (4%)	26	13
1	B	194/214 (91%)	190 (98%)	4 (2%)	47	36
1	C	191/214 (89%)	186 (97%)	5 (3%)	40	28
1	D	187/214 (87%)	181 (97%)	6 (3%)	34	22
All	All	757/856 (88%)	734 (97%)	23 (3%)	35	24

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	20	LEU
1	A	68	LEU
1	A	98	LYS
1	A	138	LEU
1	A	148	GLU
1	A	204	GLU
1	A	205	ARG
1	B	-6	LEU
1	B	20	LEU
1	B	68	LEU
1	B	231	ASP
1	C	68	LEU
1	C	94	GLN
1	C	98	LYS
1	C	134	GLN
1	C	231	ASP
1	D	62	ARG
1	D	96	VAL
1	D	148	GLU
1	D	204	GLU
1	D	205	ARG
1	D	233	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	B	84	ASN
1	B	146	GLN
1	B	171	GLN
1	C	28	HIS
1	C	69	HIS
1	C	84	ASN
1	C	94	GLN
1	C	171	GLN
1	D	84	ASN
1	D	134	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](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	B	250	-	4,4,4	0.23	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	253	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	C	252	-	4,4,4	0.24	0	6,6,6	0.19	0
2	SO4	A	252	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	B	253	-	4,4,4	0.23	0	6,6,6	0.18	0
2	SO4	A	250	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	C	250	-	4,4,4	0.19	0	6,6,6	0.20	0
2	SO4	D	252	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	B	252	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	D	250	-	4,4,4	0.24	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	252	SO4	2	0
2	B	253	SO4	1	0
2	B	252	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 [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	232/268 (86%)	-1.26	0 100 100	16, 25, 47, 71	2 (0%)
1	B	240/268 (89%)	-1.24	0 100 100	10, 25, 51, 69	4 (1%)
1	C	239/268 (89%)	-1.22	0 100 100	10, 25, 48, 75	3 (1%)
1	D	233/268 (86%)	-1.23	0 100 100	15, 24, 47, 74	3 (1%)
All	All	944/1072 (88%)	-1.24	0 100 100	10, 25, 48, 75	12 (1%)

There are no RSRZ outliers to report.

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	B	252	5/5	0.96	0.07	90,92,92,93	0
2	SO4	C	252	5/5	0.97	0.06	91,94,96,97	0
2	SO4	D	252	5/5	0.97	0.05	90,91,91,91	0
2	SO4	C	253	5/5	0.98	0.05	74,75,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	253	5/5	0.99	0.04	61,63,65,65	0
2	SO4	A	252	5/5	0.99	0.03	71,71,72,73	0
2	SO4	B	250	5/5	0.99	0.03	22,27,28,29	0
2	SO4	D	250	5/5	0.99	0.04	27,28,29,30	0
2	SO4	A	250	5/5	0.99	0.03	28,28,30,30	0
3	CL	A	253	1/1	0.99	0.07	48,48,48,48	0
3	CL	A	251	1/1	1.00	0.01	22,22,22,22	0
2	SO4	C	250	5/5	1.00	0.03	23,24,30,31	0
3	CL	B	251	1/1	1.00	0.01	25,25,25,25	0
3	CL	C	251	1/1	1.00	0.02	23,23,23,23	0
3	CL	D	251	1/1	1.00	0.01	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.