



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:47 PM UTC

PDB ID : 3A52 / pdb_00003a52
Title : Crystal structure of cold-active alkaline phosphatase from psychrophile *Shewanella* sp.
Authors : Tsuruta, H.; Mikami, B.; Higashi, T.; Aizono, Y.
Deposited on : 2009-07-24
Resolution : 2.20 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

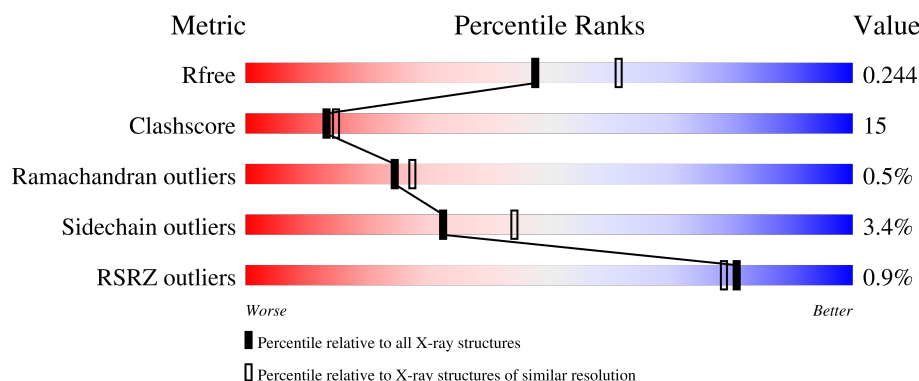
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	400	73% 24% .
1	B	400	71% 26% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6862 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 Cold-active alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3028	1897	514	602	15			
1	B	398	Total	C	N	O	S	0	0	0
			3012	1888	511	598	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8RQU7
A	2	GLY	-	expression tag	UNP Q8RQU7
B	1	MET	-	expression tag	UNP Q8RQU7
B	2	GLY	-	expression tag	UNP Q8RQU7

- 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	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0

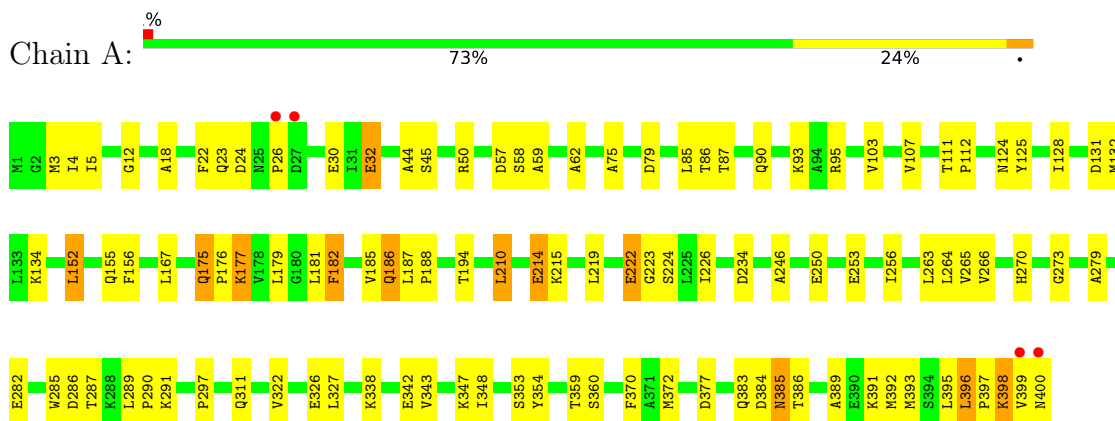
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	429	Total O 429 429	0	0
5	B	372	Total O 372 372	0	0

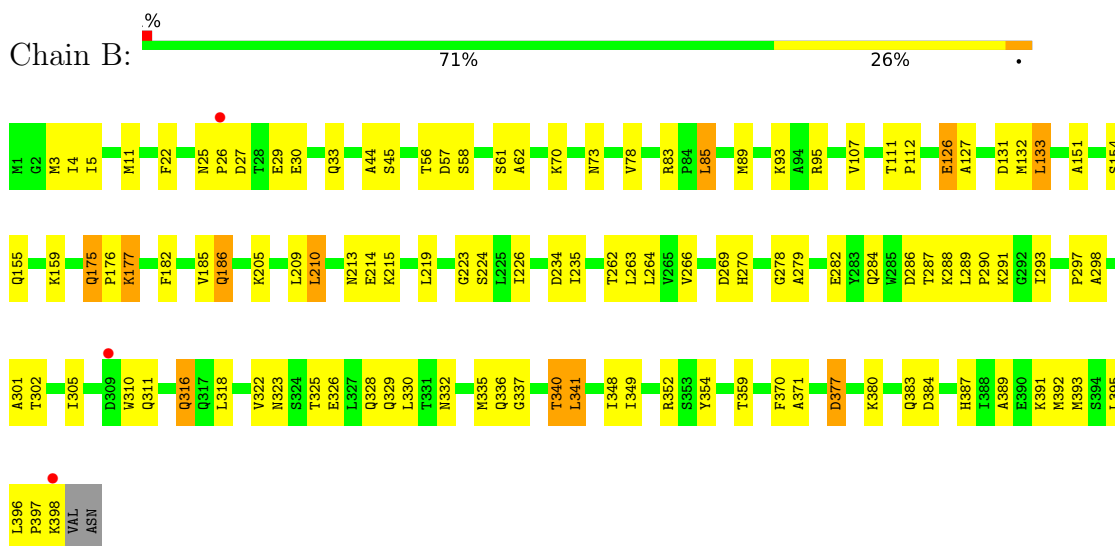
3 Residue-property plots [i](#)

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: Cold-active alkaline phosphatase



- Molecule 1: Cold-active alkaline phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.06Å 95.86Å 71.06Å 90.00° 101.62° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-2.20) 96.9 (15.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.67 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.183 , 0.244 0.183 , 0.244	Depositor DCC
R_{free} test set	4164 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6862	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.82% 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: ZN, MG, 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	0.38	0/3082	0.90	15/4184 (0.4%)
1	B	0.38	0/3066	0.91	11/4163 (0.3%)
All	All	0.38	0/6148	0.90	26/8347 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ILE	N-CA-C	-7.86	103.14	110.53
1	B	226	ILE	N-CA-C	-7.71	103.28	110.53
1	B	224	SER	N-CA-C	7.21	119.14	111.28
1	B	175	GLN	CA-C-N	7.04	127.07	119.89
1	B	175	GLN	C-N-CA	7.04	127.07	119.89
1	A	125	TYR	N-CA-C	6.29	118.70	111.02
1	B	278	GLY	N-CA-C	-6.07	103.77	111.72
1	A	57	ASP	N-CA-C	-5.81	101.58	109.95
1	A	224	SER	N-CA-C	5.77	118.51	111.82
1	B	235	ILE	N-CA-C	5.66	116.44	110.72
1	A	175	GLN	CA-C-N	5.64	125.64	119.89
1	A	175	GLN	C-N-CA	5.64	125.64	119.89
1	A	223	GLY	N-CA-C	-5.61	99.89	113.18
1	B	182	PHE	N-CA-C	5.60	119.20	112.93
1	A	396	LEU	CA-C-N	5.54	125.54	119.89
1	A	396	LEU	C-N-CA	5.54	125.54	119.89
1	A	12	GLY	CA-C-N	5.50	125.59	119.32
1	A	12	GLY	C-N-CA	5.50	125.59	119.32
1	B	57	ASP	N-CA-C	-5.49	102.04	109.95
1	B	223	GLY	N-CA-C	-5.39	100.40	113.18
1	A	360	SER	N-CA-C	-5.26	106.54	113.17
1	A	182	PHE	N-CA-C	5.14	119.19	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	GLY	N-CA-C	5.09	121.88	115.42
1	A	222	GLU	N-CA-C	5.08	117.17	108.90
1	B	11	MET	N-CA-C	5.08	117.46	109.39
1	B	337	GLY	N-CA-C	5.06	116.98	110.96

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	3028	0	2973	85	0
1	B	3012	0	2958	95	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	429	0	0	4	0
5	B	372	0	0	8	0
All	All	6862	0	5931	177	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 15.

All (177) 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:A:256:ILE:HD12	1:A:372:MET:HE3	1.38	1.04
1:A:322:VAL:HG22	1:A:326:GLU:HB2	1.48	0.95
1:A:398:LYS:HD3	1:A:398:LYS:H	1.33	0.94
1:A:253:GLU:HA	1:A:372:MET:HE1	1.48	0.93
1:B:322:VAL:HG13	1:B:326:GLU:HB2	1.48	0.93
1:A:194:THR:HG23	5:A:2190:HOH:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASP:O	1:B:290:PRO:HD3	1.78	0.83
1:A:322:VAL:CG2	1:A:326:GLU:HB2	2.09	0.83
1:B:186:GLN:NE2	1:B:186:GLN:H	1.77	0.82
1:A:286:ASP:O	1:A:290:PRO:HD3	1.81	0.81
1:A:287:THR:C	1:A:290:PRO:HD2	2.05	0.80
1:A:87:THR:H	1:A:90:GLN:HE21	1.27	0.79
1:B:325:THR:HG22	1:B:329:GLN:HE21	1.46	0.79
1:B:282:GLU:HG3	1:B:284:GLN:HG2	1.65	0.78
1:B:287:THR:C	1:B:290:PRO:HD2	2.11	0.76
1:A:398:LYS:HD3	1:A:398:LYS:N	2.01	0.75
1:B:107:VAL:O	1:B:132:MET:HE1	1.88	0.74
1:B:397:PRO:O	1:B:398:LYS:HB2	1.85	0.74
1:B:318:LEU:HD22	1:B:349:ILE:HD11	1.69	0.73
1:B:387:HIS:HB3	1:B:391:LYS:HZ2	1.55	0.72
1:B:186:GLN:H	1:B:186:GLN:HE21	1.36	0.70
1:A:286:ASP:O	1:A:290:PRO:CD	2.40	0.70
1:A:290:PRO:HG3	5:A:2527:HOH:O	1.91	0.68
1:A:385:ASN:HD22	1:A:386:THR:N	1.91	0.68
1:A:186:GLN:NE2	1:A:186:GLN:H	1.91	0.68
1:B:286:ASP:O	1:B:290:PRO:CD	2.41	0.68
1:A:253:GLU:HG2	1:A:372:MET:HE1	1.76	0.67
1:B:384:ASP:HB3	1:B:387:HIS:HD2	1.57	0.67
1:A:186:GLN:H	1:A:186:GLN:HE21	1.43	0.66
1:A:385:ASN:HD22	1:A:386:THR:H	1.42	0.66
1:A:87:THR:H	1:A:90:GLN:NE2	1.91	0.66
1:B:25:ASN:ND2	1:B:27:ASP:H	1.95	0.65
1:B:305:ILE:HG23	1:B:341:LEU:HD12	1.80	0.64
1:B:387:HIS:HB3	1:B:391:LYS:NZ	2.13	0.64
1:A:287:THR:O	1:A:290:PRO:HD2	1.97	0.63
1:B:266:VAL:HB	1:B:370:PHE:HB2	1.79	0.62
1:B:25:ASN:HD22	1:B:26:PRO:N	1.97	0.62
1:B:322:VAL:CG1	1:B:326:GLU:HB2	2.28	0.62
1:A:399:VAL:HG13	1:A:400:ASN:N	2.15	0.62
1:A:398:LYS:H	1:A:398:LYS:CD	2.11	0.61
1:B:328:GLN:HG3	5:B:2736:HOH:O	2.01	0.61
1:B:205:LYS:O	1:B:209:LEU:HD23	2.00	0.61
1:B:22:PHE:O	1:B:291:LYS:HE2	2.01	0.60
1:B:25:ASN:HD22	1:B:25:ASN:C	2.07	0.60
1:B:298:ALA:O	1:B:302:THR:HG23	2.01	0.60
1:B:213:ASN:C	1:B:213:ASN:HD22	2.08	0.60
1:A:176:PRO:O	1:A:177:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ASN:HA	1:B:335:MET:HE3	1.83	0.59
1:A:343:VAL:HG12	1:A:347:LYS:HE3	1.84	0.59
1:A:338:LYS:O	1:A:342:GLU:HG3	2.03	0.59
1:B:213:ASN:ND2	1:B:215:LYS:H	2.00	0.59
1:A:264:LEU:HD23	1:A:372:MET:HE2	1.85	0.59
1:A:107:VAL:O	1:A:132:MET:HE1	2.03	0.59
1:B:316:GLN:HE21	1:B:316:GLN:C	2.12	0.58
1:B:176:PRO:O	1:B:177:LYS:HB2	2.03	0.58
1:B:287:THR:O	1:B:290:PRO:HD2	2.04	0.57
1:B:290:PRO:HG3	5:B:2396:HOH:O	2.05	0.57
1:A:131:ASP:OD2	1:A:134:LYS:HD2	2.05	0.57
1:B:56:THR:HA	1:B:73:ASN:HD21	1.68	0.57
1:B:325:THR:HG22	1:B:329:GLN:NE2	2.19	0.57
1:A:4:ILE:HD12	1:A:4:ILE:N	2.20	0.56
1:B:186:GLN:HE21	1:B:186:GLN:N	2.02	0.56
1:B:322:VAL:HG13	1:B:326:GLU:CB	2.28	0.56
1:A:50:ARG:HD2	1:B:29:GLU:O	2.06	0.56
1:A:253:GLU:CA	1:A:372:MET:HE1	2.29	0.56
1:A:377:ASP:HB3	5:A:2688:HOH:O	2.06	0.56
1:B:397:PRO:O	1:B:398:LYS:CB	2.54	0.55
1:B:288:LYS:HD2	5:B:2554:HOH:O	2.07	0.54
1:A:103:VAL:HG12	1:A:222:GLU:HB3	1.90	0.54
1:B:377:ASP:OD2	1:B:380:LYS:HD3	2.08	0.54
1:A:234:ASP:OD2	1:A:297:PRO:HD2	2.08	0.53
1:A:322:VAL:CG2	1:A:326:GLU:CB	2.85	0.53
1:B:326:GLU:OE2	1:B:352:ARG:HD2	2.07	0.53
1:B:44:ALA:HA	1:B:383:GLN:O	2.08	0.52
1:B:282:GLU:HG2	1:B:354:TYR:CD1	2.44	0.52
1:B:70:LYS:HE2	1:B:384:ASP:OD2	2.09	0.52
1:B:25:ASN:HD22	1:B:26:PRO:CD	2.22	0.52
1:A:79:ASP:N	1:A:85:LEU:HD21	2.24	0.52
1:A:253:GLU:HG2	1:A:372:MET:CE	2.40	0.52
1:A:253:GLU:HA	1:A:372:MET:CE	2.32	0.52
1:A:5:ILE:HB	1:A:392:MET:HE1	1.92	0.52
1:B:326:GLU:HB3	1:B:348:ILE:HD13	1.92	0.51
1:A:343:VAL:O	1:A:347:LYS:HG3	2.10	0.51
1:A:44:ALA:HA	1:A:383:GLN:O	2.10	0.51
1:A:214:GLU:HG3	1:A:215:LYS:N	2.25	0.51
1:A:3:MET:HE1	1:A:392:MET:O	2.11	0.51
1:B:5:ILE:HB	1:B:392:MET:HE1	1.93	0.51
1:A:359:THR:HB	1:B:279:ALA:HA	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:HIS:O	1:B:391:LYS:HG3	2.12	0.50
1:A:95:ARG:HD3	1:A:397:PRO:HD2	1.94	0.50
1:A:266:VAL:HB	1:A:370:PHE:HB2	1.92	0.49
1:A:22:PHE:O	1:A:291:LYS:HE2	2.13	0.49
1:A:111:THR:HB	1:A:112:PRO:CD	2.42	0.49
1:B:3:MET:HE1	1:B:392:MET:O	2.12	0.49
1:A:389:ALA:O	1:A:393:MET:HG3	2.13	0.49
1:B:213:ASN:HD22	1:B:214:GLU:N	2.11	0.48
1:A:279:ALA:HA	1:B:359:THR:HB	1.94	0.48
1:B:61:SER:OG	1:B:269:ASP:HB2	2.13	0.48
1:A:246:ALA:O	1:A:250:GLU:HG2	2.13	0.48
1:A:343:VAL:CG1	1:A:347:LYS:HE3	2.44	0.48
1:A:95:ARG:HH11	1:A:95:ARG:HG3	1.79	0.47
1:A:186:GLN:HE21	1:A:186:GLN:N	2.10	0.47
1:A:263:LEU:HD22	1:A:395:LEU:CD2	2.44	0.47
1:B:111:THR:HB	1:B:112:PRO:CD	2.43	0.47
1:B:282:GLU:CD	1:B:284:GLN:HE21	2.22	0.47
1:A:86:THR:HA	1:A:90:GLN:NE2	2.29	0.47
1:B:389:ALA:O	1:B:393:MET:HG3	2.13	0.47
1:B:387:HIS:CD2	5:B:2304:HOH:O	2.67	0.47
1:B:282:GLU:HG2	1:B:354:TYR:CE1	2.49	0.47
1:B:336:GLN:CG	1:B:340:THR:HG21	2.45	0.47
1:A:289:LEU:HB3	1:A:290:PRO:HD3	1.97	0.47
1:B:263:LEU:HD22	1:B:395:LEU:CD1	2.45	0.47
1:A:187:LEU:HB3	1:A:188:PRO:HD2	1.96	0.46
1:B:336:GLN:HG2	1:B:340:THR:HG21	1.97	0.46
1:A:45:SER:OG	1:A:384:ASP:HA	2.15	0.46
1:B:301:ALA:HA	1:B:341:LEU:HD13	1.98	0.46
1:B:293:ILE:HD11	1:B:349:ILE:HD12	1.97	0.46
1:B:89:MET:O	1:B:93:LYS:HG2	2.16	0.45
1:B:83:ARG:O	1:B:85:LEU:HD13	2.16	0.45
1:B:234:ASP:OD1	1:B:297:PRO:HD2	2.17	0.45
1:B:33:GLN:NE2	5:B:2078:HOH:O	2.47	0.45
1:B:45:SER:OG	1:B:384:ASP:HA	2.16	0.45
1:B:210:LEU:CD2	1:B:219:LEU:HB2	2.46	0.45
1:B:83:ARG:NE	5:B:2584:HOH:O	2.35	0.45
1:B:284:GLN:HG3	1:B:354:TYR:CD2	2.52	0.45
1:A:282:GLU:HG3	1:A:354:TYR:CD2	2.51	0.45
1:A:385:ASN:ND2	1:A:386:THR:N	2.62	0.44
1:B:25:ASN:ND2	1:B:25:ASN:C	2.72	0.44
1:A:45:SER:HG	1:A:384:ASP:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD22	1:A:156:PHE:CE2	2.52	0.44
1:A:58:SER:OG	1:A:270:HIS:HE1	2.00	0.44
1:A:210:LEU:HD23	1:A:219:LEU:HB2	2.00	0.44
1:B:262:THR:HG22	1:B:263:LEU:N	2.32	0.44
1:B:30:GLU:OE2	1:B:30:GLU:N	2.35	0.44
1:B:4:ILE:HD12	1:B:4:ILE:N	2.32	0.44
1:A:282:GLU:HG3	1:A:354:TYR:CE2	2.53	0.44
1:B:186:GLN:NE2	1:B:186:GLN:N	2.56	0.44
1:B:398:LYS:HE3	5:B:2493:HOH:O	2.18	0.44
1:A:326:GLU:HB3	1:A:348:ILE:HD13	1.99	0.43
1:A:399:VAL:CG1	1:A:400:ASN:N	2.81	0.43
1:B:78:VAL:HA	1:B:83:ARG:O	2.18	0.43
1:B:301:ALA:O	1:B:305:ILE:HG12	2.18	0.43
1:A:18:ALA:HB1	1:A:285:TRP:CH2	2.52	0.43
1:A:311:GLN:HE22	1:A:327:LEU:HD22	1.83	0.43
1:B:332:ASN:HA	1:B:335:MET:CE	2.47	0.43
1:A:264:LEU:HD12	1:A:265:VAL:N	2.34	0.43
1:A:30:GLU:OE1	1:A:32:GLU:OE1	2.37	0.43
1:B:323:ASN:OD1	1:B:326:GLU:HG3	2.19	0.42
1:A:24:ASP:O	1:A:26:PRO:HD3	2.19	0.42
1:A:155:GLN:HG2	5:A:2657:HOH:O	2.18	0.42
1:A:286:ASP:HB3	1:A:353:SER:HA	2.00	0.42
1:A:311:GLN:NE2	1:A:327:LEU:HD13	2.33	0.42
1:A:59:ALA:HB1	1:A:75:ALA:O	2.19	0.42
1:B:62:ALA:CB	1:B:111:THR:HA	2.48	0.42
1:A:3:MET:C	1:A:4:ILE:HD12	2.45	0.42
1:B:133:LEU:HD11	1:B:155:GLN:HB3	2.02	0.42
1:B:326:GLU:O	1:B:330:LEU:HG	2.20	0.42
1:A:167:LEU:HD23	1:A:182:PHE:CD2	2.55	0.42
1:B:83:ARG:NH1	5:B:2782:HOH:O	2.53	0.42
1:B:213:ASN:C	1:B:213:ASN:ND2	2.74	0.41
1:B:264:LEU:O	1:B:371:ALA:HA	2.19	0.41
1:B:126:GLU:HG2	1:B:127:ALA:N	2.34	0.41
1:B:175:GLN:NE2	1:B:176:PRO:HD2	2.36	0.41
1:B:58:SER:OG	1:B:270:HIS:HE1	2.03	0.41
1:A:62:ALA:CB	1:A:111:THR:HA	2.51	0.41
1:B:151:ALA:O	1:B:154:SER:HB3	2.21	0.41
1:A:287:THR:CA	1:A:290:PRO:HD2	2.49	0.41
1:B:133:LEU:HD22	1:B:159:LYS:CD	2.51	0.41
1:B:316:GLN:C	1:B:316:GLN:NE2	2.79	0.41
1:A:22:PHE:HD1	1:A:23:GLN:HE21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:N	1:A:85:LEU:CD2	2.84	0.40
1:A:93:LYS:HD3	1:A:93:LYS:HA	1.98	0.40
1:A:124:ASN:O	1:A:128:ILE:HG13	2.22	0.40
1:B:310:TRP:CE2	1:B:311:GLN:NE2	2.90	0.40
1:B:95:ARG:HG3	1:B:95:ARG:HH11	1.86	0.40
1:A:175:GLN:HA	1:A:176:PRO:HD3	1.93	0.40
1:B:289:LEU:HB3	1:B:290:PRO:HD3	2.03	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	398/400 (100%)	386 (97%)	10 (2%)	2 (0%)	24	27
1	B	396/400 (99%)	380 (96%)	14 (4%)	2 (0%)	24	27
All	All	794/800 (99%)	766 (96%)	24 (3%)	4 (0%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	LYS
1	B	177	LYS
1	A	185	VAL
1	B	185	VAL

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	320/320 (100%)	309 (97%)	11 (3%)	32	44
1	B	318/320 (99%)	307 (96%)	11 (4%)	32	43
All	All	638/640 (100%)	616 (97%)	22 (3%)	32	44

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	152	LEU
1	A	179	LEU
1	A	181	LEU
1	A	186	GLN
1	A	210	LEU
1	A	214	GLU
1	A	385	ASN
1	A	391	LYS
1	A	396	LEU
1	A	398	LYS
1	B	85	LEU
1	B	126	GLU
1	B	131	ASP
1	B	133	LEU
1	B	186	GLN
1	B	210	LEU
1	B	316	GLN
1	B	340	THR
1	B	341	LEU
1	B	377	ASP
1	B	396	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	33	GLN
1	A	81	ASN
1	A	90	GLN
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	197	ASN
1	A	232	ASN
1	A	233	ASN
1	A	243	GLN
1	A	254	GLN
1	A	311	GLN
1	A	328	GLN
1	A	329	GLN
1	A	332	ASN
1	A	382	ASN
1	A	385	ASN
1	B	23	GLN
1	B	25	ASN
1	B	73	ASN
1	B	109	HIS
1	B	124	ASN
1	B	175	GLN
1	B	186	GLN
1	B	197	ASN
1	B	204	GLN
1	B	213	ASN
1	B	233	ASN
1	B	303	HIS
1	B	315	ASN
1	B	316	GLN
1	B	329	GLN
1	B	332	ASN
1	B	336	GLN
1	B	387	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	3005	3	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	A	3004	3	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	B	3003	-	4,4,4	0.34	0	6,6,6	0.11	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	400/400 (100%)	-0.32	4 (1%) 79 77	3, 9, 24, 39	0
1	B	398/400 (99%)	-0.34	3 (0%) 82 80	3, 10, 25, 34	0
All	All	798/800 (99%)	-0.33	7 (0%) 81 79	3, 9, 24, 39	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	PRO	3.9
1	A	400	ASN	3.9
1	A	399	VAL	3.4
1	B	309	ASP	2.4
1	A	27	ASP	2.3
1	B	26	PRO	2.1
1	B	398	LYS	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	3005	5/5	0.95	0.10	32,32,34,36	0
4	MG	A	1003	1/1	0.95	0.05	28,28,28,28	0
2	SO4	A	3004	5/5	0.96	0.12	22,23,25,27	0
2	SO4	B	3003	5/5	0.96	0.07	33,33,34,34	0
4	MG	B	1006	1/1	0.96	0.06	29,29,29,29	0
4	MG	A	1007	1/1	0.99	0.05	1,1,1,1	0
4	MG	B	1008	1/1	0.99	0.06	1,1,1,1	0
3	ZN	A	1001	1/1	1.00	0.04	12,12,12,12	0
3	ZN	B	1004	1/1	1.00	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.