



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:10 PM UTC

PDB ID : 2D73 / pdb_00002d73
Title : Crystal Structure Analysis of SusB
Authors : Kitamura, M.; Yao, M.
Deposited on : 2005-11-15
Resolution : 1.60 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
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

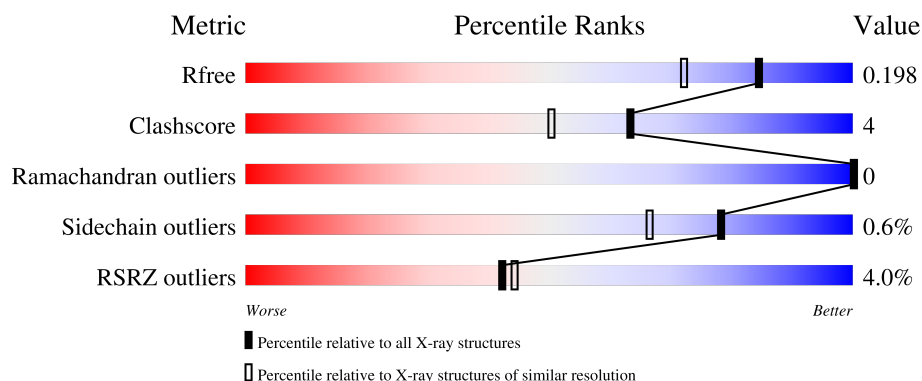
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	738	
1	B	738	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12992 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 alpha-glucosidase SusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	717	Total	C	N	O	S	0	0	0
			5784	3671	977	1108	28			
1	B	717	Total	C	N	O	S	0	0	0
			5784	3671	977	1108	28			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	GB 29341018
A	2	GLY	-	expression tag	GB 29341018
A	3	SER	-	expression tag	GB 29341018
A	4	SER	-	expression tag	GB 29341018
A	5	HIS	-	expression tag	GB 29341018
A	6	HIS	-	expression tag	GB 29341018
A	7	HIS	-	expression tag	GB 29341018
A	8	HIS	-	expression tag	GB 29341018
A	9	HIS	-	expression tag	GB 29341018
A	10	HIS	-	expression tag	GB 29341018
A	11	SER	-	expression tag	GB 29341018
A	12	SER	-	expression tag	GB 29341018
A	13	GLY	-	expression tag	GB 29341018
A	14	LEU	-	expression tag	GB 29341018
A	15	VAL	-	expression tag	GB 29341018
A	16	PRO	-	expression tag	GB 29341018
A	17	ARG	-	expression tag	GB 29341018
A	18	GLY	-	expression tag	GB 29341018
A	19	SER	-	expression tag	GB 29341018
A	20	HIS	-	expression tag	GB 29341018
A	21	MET	-	expression tag	GB 29341018
B	1	MET	-	expression tag	GB 29341018
B	2	GLY	-	expression tag	GB 29341018
B	3	SER	-	expression tag	GB 29341018
B	4	SER	-	expression tag	GB 29341018

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	GB 29341018
B	6	HIS	-	expression tag	GB 29341018
B	7	HIS	-	expression tag	GB 29341018
B	8	HIS	-	expression tag	GB 29341018
B	9	HIS	-	expression tag	GB 29341018
B	10	HIS	-	expression tag	GB 29341018
B	11	SER	-	expression tag	GB 29341018
B	12	SER	-	expression tag	GB 29341018
B	13	GLY	-	expression tag	GB 29341018
B	14	LEU	-	expression tag	GB 29341018
B	15	VAL	-	expression tag	GB 29341018
B	16	PRO	-	expression tag	GB 29341018
B	17	ARG	-	expression tag	GB 29341018
B	18	GLY	-	expression tag	GB 29341018
B	19	SER	-	expression tag	GB 29341018
B	20	HIS	-	expression tag	GB 29341018
B	21	MET	-	expression tag	GB 29341018

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

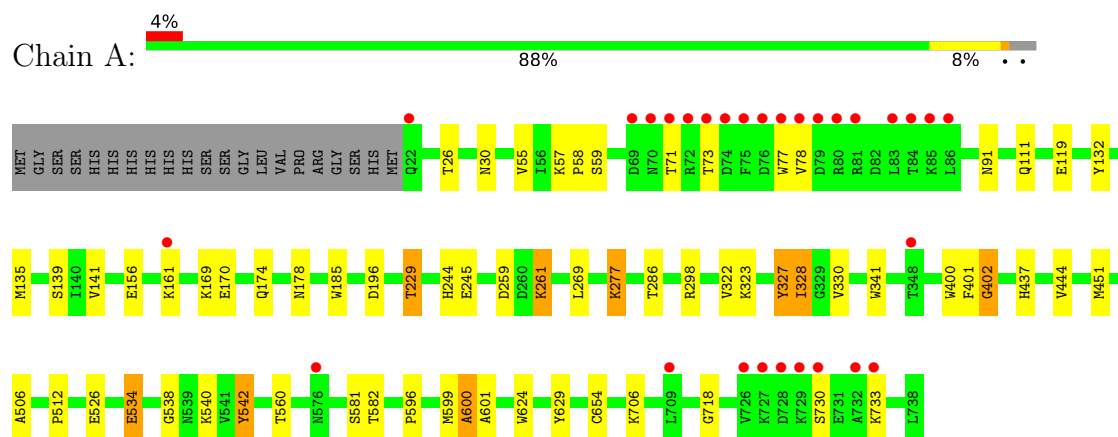
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	699	Total O 699 699	0	0
3	B	723	Total O 723 723	0	0

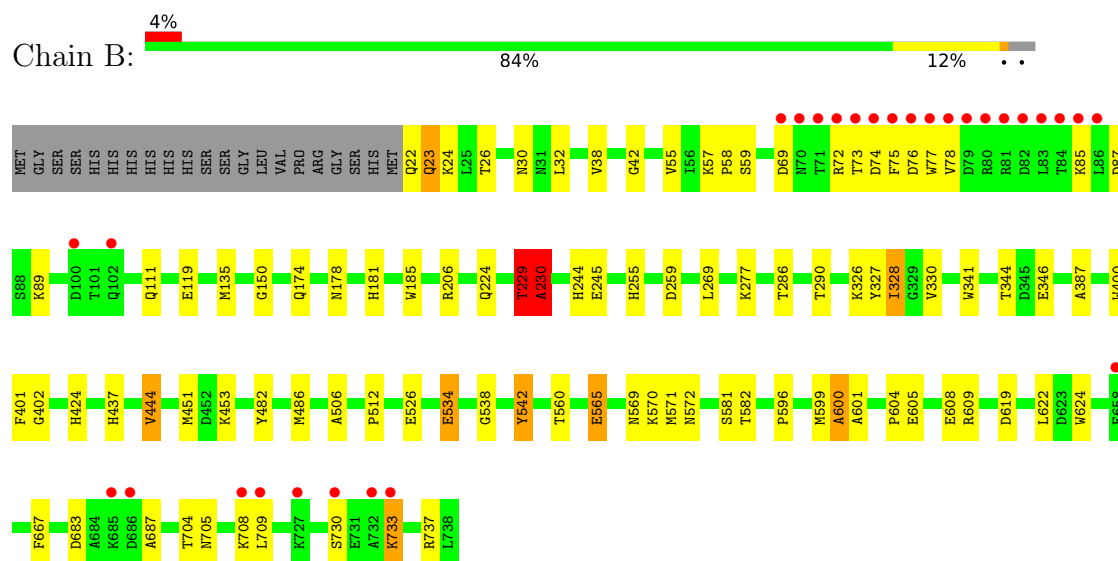
3 Residue-property plots [i](#)

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: alpha-glucosidase SusB



• Molecule 1: alpha-glucosidase SusB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.63Å 112.34Å 102.57Å 90.00° 100.65° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 15.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.9 (15.00-1.60) 99.6 (15.00-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.198 0.176 , 0.198	Depositor DCC
R_{free} test set	21923 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12992	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: CA

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	0.33	1/5935 (0.0%)	0.92	26/8048 (0.3%)
1	B	0.35	2/5935 (0.0%)	0.94	31/8048 (0.4%)
All	All	0.34	3/11870 (0.0%)	0.93	57/16096 (0.4%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	ALA	N-CA	7.87	1.61	1.46
1	B	560	THR	CA-CB	6.28	1.57	1.52
1	A	560	THR	CA-CB	5.73	1.56	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	THR	O-C-N	-13.41	107.88	123.03
1	B	229	THR	CA-C-N	10.38	140.38	121.70
1	B	229	THR	C-N-CA	10.38	140.38	121.70
1	B	229	THR	CA-C-O	9.72	132.75	121.28
1	A	401	PHE	N-CA-C	8.36	122.14	108.52
1	B	601	ALA	N-CA-C	8.12	122.45	112.54
1	B	451	MET	N-CA-C	8.10	119.73	111.07
1	A	451	MET	N-CA-C	7.88	119.50	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	601	ALA	N-CA-C	7.85	122.12	112.54
1	B	401	PHE	N-CA-C	7.76	121.72	107.99
1	A	444	VAL	N-CA-C	7.48	119.16	111.00
1	B	526	GLU	N-CA-C	-7.08	95.72	110.80
1	B	444	VAL	N-CA-C	7.02	118.65	111.00
1	A	526	GLU	N-CA-C	-6.99	95.91	110.80
1	B	600	ALA	N-CA-C	-6.75	94.33	107.62
1	B	286	THR	N-CA-C	-6.72	102.40	110.13
1	B	330	VAL	N-CA-C	-6.71	97.83	107.37
1	B	185	TRP	N-CA-C	6.59	119.19	109.24
1	A	261	LYS	N-CA-C	-6.48	105.02	113.12
1	A	600	ALA	N-CA-C	-6.41	94.46	107.41
1	A	286	THR	N-CA-C	-6.38	102.79	110.13
1	A	185	TRP	N-CA-C	6.29	118.74	109.24
1	B	624	TRP	N-CA-C	6.20	119.30	109.50
1	B	506	ALA	N-CA-C	5.98	118.43	108.20
1	A	330	VAL	N-CA-C	-5.98	98.88	107.37
1	A	259	ASP	N-CA-C	-5.97	97.48	107.99
1	A	624	TRP	N-CA-C	5.97	118.93	109.50
1	A	328	ILE	N-CA-C	-5.86	101.67	108.82
1	B	259	ASP	N-CA-C	-5.84	97.70	107.99
1	A	55	VAL	N-CA-C	-5.84	106.53	111.56
1	A	506	ALA	N-CA-C	5.81	118.13	108.20
1	B	402	GLY	N-CA-C	5.79	123.24	114.61
1	B	596	PRO	N-CA-C	-5.75	107.17	114.35
1	A	402	GLY	N-CA-C	5.72	123.14	114.61
1	A	534	GLU	N-CA-C	-5.70	106.17	113.01
1	B	400	TRP	N-CA-C	5.70	119.33	112.38
1	B	582	THR	N-CA-C	-5.68	102.06	110.46
1	A	277	LYS	N-CA-C	5.46	119.11	111.30
1	B	328	ILE	N-CA-C	-5.44	102.18	108.82
1	B	55	VAL	N-CA-C	-5.41	106.91	111.56
1	B	512	PRO	N-CA-C	5.30	119.65	111.21
1	B	534	GLU	N-CA-C	-5.29	106.67	113.01
1	B	230	ALA	N-CA-C	-5.27	96.23	111.00
1	B	619	ASP	N-CA-C	5.25	118.15	111.69
1	A	341	TRP	N-CA-C	-5.24	105.63	112.23
1	B	290	THR	N-CA-C	5.23	117.92	109.40
1	A	596	PRO	N-CA-C	-5.19	107.26	114.27
1	B	255	HIS	N-CA-C	-5.17	102.24	109.69
1	B	482	TYR	N-CA-C	5.11	118.82	112.59
1	B	150	GLY	N-CA-C	5.11	117.88	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	THR	N-CA-C	-5.08	102.94	110.46
1	A	229	THR	CA-C-O	5.08	127.85	121.66
1	B	387	ALA	N-CA-C	5.07	116.52	108.96
1	A	400	TRP	N-CA-C	5.05	118.70	112.54
1	A	512	PRO	N-CA-C	5.05	119.24	111.21
1	A	327	TYR	N-CA-C	5.04	116.65	109.14
1	B	341	TRP	N-CA-C	-5.01	105.92	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5552	33	0
1	B	5784	0	5552	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	699	0	0	5	0
3	B	723	0	0	7	0
All	All	12992	0	11104	90	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 4.

All (90) 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:453:LYS:HA	1:B:453:LYS:HE2	1.43	0.98
1:B:73:THR:HG21	1:B:77:TRP:HA	1.55	0.88
1:A:730:SER:HA	1:A:733:LYS:HE3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLN:HG2	1:B:119:GLU:HG2	1.74	0.70
1:B:534:GLU:HA	1:B:538:GLY:HA2	1.74	0.68
1:B:73:THR:HG22	1:B:74:ASP:O	1.94	0.68
1:A:534:GLU:HA	1:A:538:GLY:HA2	1.75	0.67
1:A:111:GLN:HG2	1:A:119:GLU:HG2	1.79	0.62
1:B:733:LYS:HE3	1:B:733:LYS:HA	1.82	0.61
1:B:73:THR:CG2	1:B:77:TRP:HA	2.28	0.61
1:B:22:GLN:HE21	1:B:24:LYS:HE2	1.68	0.59
1:B:453:LYS:HA	1:B:453:LYS:CE	2.27	0.58
1:A:57:LYS:HD2	1:A:178:ASN:HD22	1.70	0.56
1:B:708:LYS:C	1:B:709:LEU:HD12	2.31	0.55
1:B:206:ARG:HG3	1:B:224:GLN:HG2	1.89	0.55
1:B:73:THR:HG21	1:B:77:TRP:CA	2.31	0.55
1:B:604:PRO:O	1:B:608:GLU:HG3	2.05	0.55
1:B:667:PHE:HE2	1:B:709:LEU:HD13	1.72	0.55
1:B:565:GLU:HG2	1:B:609:ARG:NH1	2.20	0.55
1:A:261:LYS:C	1:A:261:LYS:HD3	2.33	0.54
1:A:402:GLY:CA	1:B:72:ARG:HH21	2.20	0.54
1:B:23:GLN:N	1:B:23:GLN:NE2	2.56	0.53
1:A:437:HIS:HD2	3:A:1041:HOH:O	1.92	0.52
1:B:181:HIS:HD2	3:B:1345:HOH:O	1.92	0.52
1:B:704:THR:HG23	1:B:737:ARG:HH12	1.74	0.52
1:B:733:LYS:HE3	1:B:733:LYS:CA	2.40	0.52
1:B:73:THR:HG23	1:B:78:VAL:N	2.24	0.52
1:B:327:TYR:CZ	1:B:599:MET:HB2	2.45	0.52
1:B:667:PHE:CE2	1:B:709:LEU:HD13	2.44	0.51
1:B:327:TYR:CE2	1:B:599:MET:HB2	2.45	0.51
1:A:581:SER:HB2	3:A:1454:HOH:O	2.11	0.50
1:B:581:SER:HB2	3:B:1363:HOH:O	2.12	0.50
1:A:261:LYS:HD3	1:A:261:LYS:O	2.12	0.50
1:B:85:LYS:O	1:B:89:LYS:HG3	2.12	0.50
1:B:344:THR:OG1	1:B:346:GLU:HG2	2.12	0.50
1:B:59:SER:HB3	1:B:174:GLN:HB2	1.93	0.49
1:B:38:VAL:CG1	1:B:42:GLY:HA2	2.43	0.49
1:B:181:HIS:HE1	3:B:1154:HOH:O	1.98	0.47
1:A:59:SER:HB3	1:A:174:GLN:HB2	1.96	0.47
1:B:565:GLU:CD	1:B:570:LYS:HD2	2.40	0.47
1:A:244:HIS:CG	1:A:245:GLU:H	2.33	0.46
1:A:161:LYS:HD2	3:A:2003:HOH:O	2.16	0.46
1:B:76:ASP:O	1:B:77:TRP:HB2	2.16	0.46
1:B:244:HIS:CG	1:B:245:GLU:H	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:O	1:A:170:GLU:HG2	2.17	0.45
1:B:667:PHE:O	1:B:705:ASN:HA	2.16	0.45
1:B:229:THR:HA	1:B:230:ALA:C	2.42	0.45
1:A:196:ASP:CG	1:A:540:LYS:HG2	2.42	0.45
1:B:605:GLU:HG3	3:B:1595:HOH:O	2.17	0.45
1:A:269:LEU:HB2	1:A:277:LYS:HD3	1.99	0.44
1:B:69:ASP:OD1	1:B:72:ARG:HD3	2.17	0.44
1:B:74:ASP:OD1	1:B:75:PHE:N	2.48	0.44
1:B:69:ASP:OD1	1:B:72:ARG:HB2	2.18	0.44
1:B:437:HIS:HD2	3:B:1053:HOH:O	2.00	0.44
1:A:73:THR:OG1	1:A:78:VAL:N	2.51	0.43
1:A:542:TYR:C	1:A:542:TYR:CD2	2.96	0.43
1:A:73:THR:OG1	1:A:77:TRP:C	2.60	0.43
1:A:132:TYR:HD1	1:A:139:SER:HG	1.66	0.43
1:B:565:GLU:OE1	1:B:570:LYS:HD2	2.18	0.43
1:B:683:ASP:HB3	1:B:687:ALA:HB3	1.99	0.43
1:B:73:THR:CG2	1:B:77:TRP:CA	2.95	0.43
1:A:298:ARG:HD2	1:A:629:TYR:O	2.19	0.43
1:B:26:THR:CG2	1:B:30:ASN:HA	2.49	0.43
1:A:91:ASN:OD1	1:A:91:ASN:C	2.62	0.43
1:B:57:LYS:HD2	1:B:178:ASN:HD22	1.83	0.43
1:B:444:VAL:HG21	1:B:486:MET:SD	2.59	0.43
1:A:327:TYR:CZ	1:A:599:MET:HB2	2.54	0.42
1:B:85:LYS:HE3	1:B:135:MET:O	2.19	0.42
1:A:57:LYS:O	1:A:58:PRO:C	2.63	0.42
1:B:542:TYR:CD1	1:B:542:TYR:C	2.98	0.42
1:B:730:SER:HA	1:B:733:LYS:HD2	2.01	0.42
1:A:111:GLN:CG	1:A:119:GLU:HG2	2.49	0.42
1:A:135:MET:HG2	3:A:1378:HOH:O	2.19	0.42
1:B:57:LYS:O	1:B:58:PRO:C	2.61	0.42
1:B:326:LYS:HB2	1:B:622:LEU:HD11	2.02	0.42
1:A:328:ILE:HG22	1:A:600:ALA:HB3	2.01	0.42
1:A:26:THR:CG2	1:A:30:ASN:HA	2.50	0.41
1:A:706:LYS:NZ	3:A:1295:HOH:O	2.53	0.41
1:B:38:VAL:HG12	1:B:42:GLY:HA2	2.00	0.41
1:B:328:ILE:HG22	1:B:600:ALA:HB3	2.03	0.41
1:B:424:HIS:HD2	3:B:1247:HOH:O	2.03	0.41
1:A:71:THR:O	1:A:71:THR:HG23	2.21	0.41
1:A:542:TYR:C	1:A:542:TYR:HD2	2.28	0.41
1:B:569:ASN:HA	1:B:572:ASN:O	2.21	0.41
1:B:571:MET:HG2	3:B:1511:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:HB	1:A:156:GLU:HB2	2.03	0.41
1:A:322:VAL:C	1:A:323:LYS:HG3	2.46	0.40
1:A:654:CYS:O	1:A:718:GLY:HA3	2.21	0.40
1:B:32:LEU:HD12	1:B:32:LEU:N	2.36	0.40
1:B:269:LEU:HB2	1:B:277:LYS:HD3	2.02	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	715/738 (97%)	688 (96%)	27 (4%)	0	100	100
1	B	715/738 (97%)	691 (97%)	24 (3%)	0	100	100
All	All	1430/1476 (97%)	1379 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	618/636 (97%)	616 (100%)	2 (0%)	86	78
1	B	618/636 (97%)	612 (99%)	6 (1%)	68	50
All	All	1236/1272 (97%)	1228 (99%)	8 (1%)	78	66

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	THR
1	A	542	TYR
1	B	23	GLN
1	B	87	ASP
1	B	229	THR
1	B	542	TYR
1	B	565	GLU
1	B	733	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	31	ASN
1	A	37	GLN
1	A	70	ASN
1	A	164	ASN
1	A	178	ASN
1	A	299	ASN
1	A	437	HIS
1	A	446	ASN
1	A	473	ASN
1	A	675	GLN
1	A	715	ASN
1	B	22	GLN
1	B	23	GLN
1	B	30	ASN
1	B	31	ASN
1	B	37	GLN
1	B	122	ASN
1	B	178	ASN
1	B	181	HIS
1	B	255	HIS
1	B	285	ASN
1	B	299	ASN
1	B	424	HIS
1	B	437	HIS
1	B	578	GLN
1	B	628	ASN
1	B	715	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	717/738 (97%)	-0.10	29 (4%)	42 44	7, 16, 32, 58	0
1	B	717/738 (97%)	-0.07	29 (4%)	42 44	6, 15, 31, 68	0
All	All	1434/1476 (97%)	-0.08	58 (4%)	42 44	6, 15, 31, 68	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	VAL	6.6
1	B	77	TRP	5.8
1	A	77	TRP	5.4
1	B	83	LEU	4.8
1	B	69	ASP	4.8
1	A	728	ASP	4.6
1	A	73	THR	4.6
1	A	78	VAL	4.3
1	A	83	LEU	4.2
1	B	72	ARG	4.1
1	B	75	PHE	4.1
1	B	73	THR	4.0
1	B	85	LYS	4.0
1	B	70	ASN	3.7
1	B	80	ARG	3.7
1	B	71	THR	3.7
1	B	74	ASP	3.6
1	A	70	ASN	3.5
1	B	84	THR	3.4
1	A	733	LYS	3.3
1	A	732	ALA	3.1
1	A	84	THR	3.0
1	A	81	ARG	3.0
1	A	75	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	82	ASP	2.9
1	A	730	SER	2.9
1	A	72	ARG	2.8
1	B	79	ASP	2.8
1	B	81	ARG	2.7
1	A	74	ASP	2.7
1	A	79	ASP	2.7
1	A	80	ARG	2.6
1	B	730	SER	2.6
1	B	727	LYS	2.6
1	A	709	LEU	2.5
1	B	733	LYS	2.5
1	B	76	ASP	2.5
1	A	86	LEU	2.4
1	B	686	ASP	2.4
1	A	161	LYS	2.4
1	A	727	LYS	2.4
1	B	685	LYS	2.4
1	B	102	GLN	2.4
1	B	709	LEU	2.4
1	A	85	LYS	2.3
1	A	69	ASP	2.3
1	B	100	ASP	2.3
1	A	71	THR	2.3
1	B	732	ALA	2.3
1	A	576	ASN	2.3
1	A	726	VAL	2.2
1	A	348	THR	2.2
1	B	86	LEU	2.2
1	A	76	ASP	2.1
1	A	729	LYS	2.1
1	B	708	LYS	2.1
1	A	22	GLN	2.1
1	B	658	GLU	2.0

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

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	CA	A	801	1/1	1.00	0.01	10,10,10,10	1
2	CA	B	802	1/1	1.00	0.01	9,9,9,9	1

6.5 Other polymers [i](#)

There are no such residues in this entry.