



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:47 PM UTC

PDB ID : 1SNZ / pdb_00001snz
Title : Crystal structure of apo human galactose mutarotase
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Deposited on : 2004-03-12
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
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

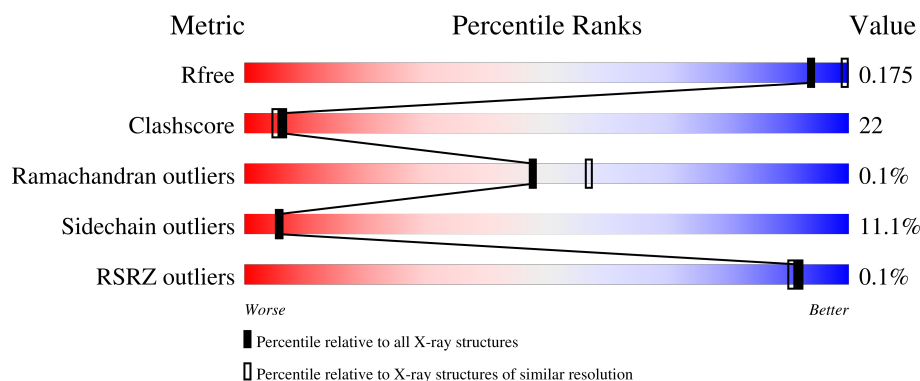
1 Overall quality at a glance

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	344	 62% 29% 6% .
1	B	344	 54% 35% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5639 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 aldose 1-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	3	0
			2704	1721	475	503	5			
1	B	342	Total	C	N	O	S	0	1	0
			2677	1707	465	500	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q96C23
A	0	HIS	-	cloning artifact	UNP Q96C23
B	-1	GLY	-	cloning artifact	UNP Q96C23
B	0	HIS	-	cloning artifact	UNP Q96C23

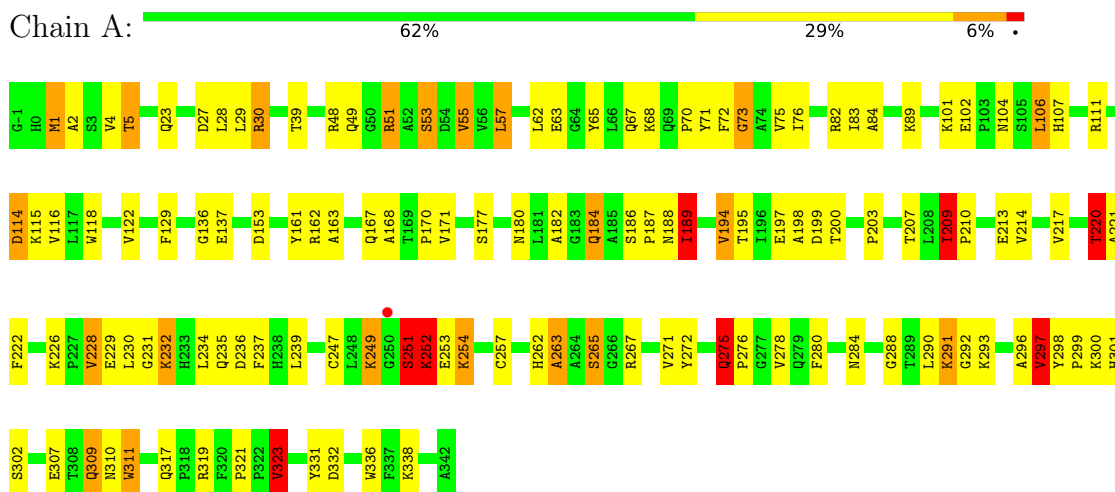
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	137	Total	O	0	0
			137	137		
2	B	121	Total	O	0	0
			121	121		

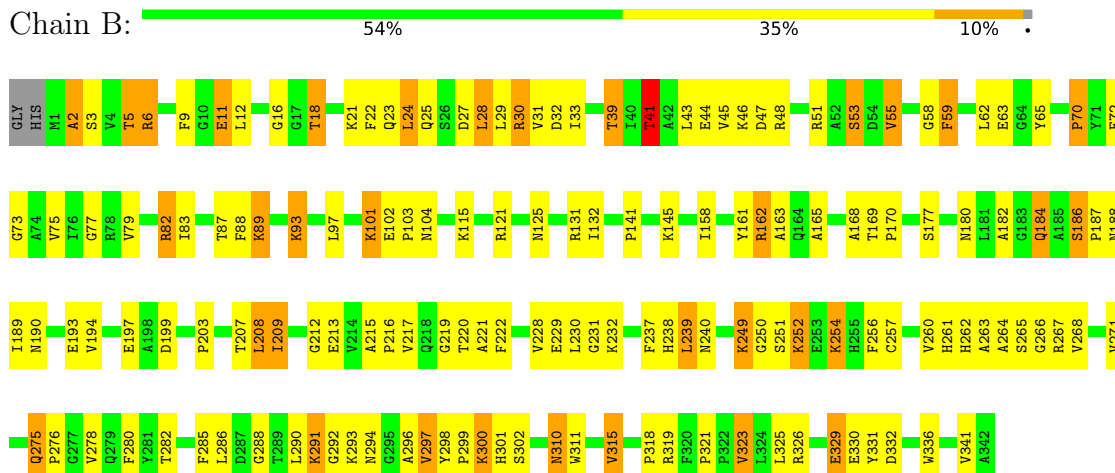
3 Residue-property plots

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: aldose 1-epimerase



• Molecule 1: aldose 1-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.70Å 90.70Å 70.00Å 90.00° 102.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-2.20) 92.7 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 2.05Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.172 , 0.201 0.172 , 0.175	Depositor DCC
R_{free} test set	4358 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.5	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	5639	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% 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

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	1.10	1/2788 (0.0%)	1.55	28/3787 (0.7%)
1	B	1.07	1/2752 (0.0%)	1.55	26/3740 (0.7%)
All	All	1.08	2/5540 (0.0%)	1.55	54/7527 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	THR	CB-OG1	6.16	1.53	1.43
1	B	5	THR	CB-OG1	5.03	1.51	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	VAL	CB-CA-C	-9.76	100.19	110.93
1	A	189	ILE	N-CA-CB	-9.33	100.23	112.36
1	A	251	SER	N-CA-C	-9.14	94.26	109.80
1	A	55	VAL	N-CA-C	8.93	120.69	112.29
1	B	323	VAL	CB-CA-C	-8.73	101.32	110.93
1	B	297	VAL	CA-C-N	-8.22	109.92	122.42
1	B	297	VAL	C-N-CA	-8.22	109.92	122.42
1	B	41	THR	N-CA-CB	-7.40	99.23	110.33
1	A	220	THR	N-CA-CB	-7.18	99.50	110.42
1	A	252	LYS	N-CA-C	-7.07	104.69	113.38
1	B	55	VAL	N-CA-C	6.94	120.78	112.80
1	B	59	PHE	CA-CB-CG	-6.76	107.04	113.80
1	B	285	PHE	CA-CB-CG	-6.47	107.33	113.80
1	B	321	PRO	N-CA-CB	6.36	106.75	103.19
1	A	280	PHE	CA-CB-CG	-6.30	107.50	113.80
1	A	311	TRP	N-CA-C	6.08	116.59	109.60
1	A	71	TYR	N-CA-C	6.04	120.23	112.86
1	B	2	ALA	N-CA-C	6.03	118.97	110.23
1	A	263	ALA	N-CA-C	6.01	117.83	111.28
1	B	3	SER	N-CA-C	-5.93	100.23	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	N-CA-C	5.86	119.63	110.32
1	B	315	VAL	CB-CA-C	-5.83	101.72	111.29
1	A	297	VAL	CA-C-N	-5.81	111.72	122.06
1	A	297	VAL	C-N-CA	-5.81	111.72	122.06
1	B	82	ARG	N-CA-C	5.77	119.49	110.32
1	A	39	THR	N-CA-C	5.73	118.02	109.25
1	B	252	LYS	N-CA-C	-5.72	104.88	112.94
1	B	280	PHE	CA-CB-CG	-5.67	108.13	113.80
1	B	310	ASN	N-CA-C	-5.64	102.18	110.52
1	A	194	VAL	N-CA-C	5.59	117.47	108.85
1	A	75	VAL	N-CA-CB	5.59	116.62	110.53
1	B	250	GLY	N-CA-C	5.58	118.73	110.42
1	B	18	THR	CA-C-N	-5.57	115.92	122.93
1	B	18	THR	C-N-CA	-5.57	115.92	122.93
1	B	70	PRO	N-CA-CB	5.55	106.45	102.28
1	B	282	THR	N-CA-C	5.52	118.81	112.57
1	A	321	PRO	N-CA-CB	5.50	108.41	103.08
1	B	141	PRO	CB-CA-C	-5.47	102.81	110.63
1	A	309	GLN	N-CA-CB	-5.45	103.02	111.35
1	A	55	VAL	N-CA-CB	-5.44	104.16	112.15
1	A	2	ALA	N-CA-C	5.43	117.69	110.53
1	B	238	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	265	SER	N-CA-C	-5.36	107.11	113.97
1	A	184	GLN	CA-CB-CG	-5.32	103.47	114.10
1	A	209	ILE	CB-CA-C	5.30	115.27	110.13
1	B	39	THR	N-CA-C	5.29	118.17	109.76
1	B	77	GLY	CA-C-O	-5.26	116.47	121.62
1	A	114	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	275	GLN	CA-C-N	5.20	125.65	120.04
1	A	275	GLN	C-N-CA	5.20	125.65	120.04
1	A	309	GLN	CB-CA-C	-5.19	101.55	112.82
1	B	256	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	212	GLY	N-CA-C	-5.13	108.38	114.48
1	A	291	LYS	N-CA-CB	-5.12	103.21	110.58

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	2704	0	2629	105	0
1	B	2677	0	2605	129	0
2	A	137	0	0	3	0
2	B	121	0	0	5	0
All	All	5639	0	5234	234	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 22.

All (234) 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:220:THR:HG22	1:B:222:PHE:H	1.03	1.13
1:A:220:THR:HG22	1:A:222:PHE:H	1.22	1.05
1:B:220:THR:HG22	1:B:222:PHE:N	1.86	0.90
1:A:189:ILE:CG2	1:A:230:LEU:HD23	2.10	0.81
1:B:162:ARG:HG2	1:B:162:ARG:HH11	1.47	0.80
1:B:53:SER:HB2	1:B:267:ARG:NH2	1.98	0.79
1:B:326:ARG:O	1:B:329:GLU:HG3	1.83	0.78
1:A:53:SER:HB2	1:A:267:ARG:NH2	1.98	0.78
1:A:73:GLY:HA2	1:A:177:SER:HA	1.65	0.78
1:A:220:THR:HG22	1:A:222:PHE:N	2.00	0.76
1:A:84:ALA:HB2	1:A:209:ILE:HD13	1.68	0.76
1:A:217:VAL:O	1:A:220:THR:HB	1.86	0.74
1:A:220:THR:CG2	1:A:222:PHE:H	1.99	0.73
1:B:131:ARG:HG2	1:B:132:ILE:N	2.02	0.73
1:B:184:GLN:OE1	1:B:293:LYS:HB2	1.88	0.73
1:B:217:VAL:O	1:B:220:THR:HB	1.89	0.72
1:A:220:THR:HG23	1:A:222:PHE:HD1	1.55	0.71
1:A:252:LYS:H	1:A:252:LYS:HD2	1.54	0.71
1:B:300:LYS:HE2	1:B:301:HIS:CE1	2.26	0.71
1:A:197:GLU:HG2	1:A:249:LYS:HE3	1.73	0.70
1:A:189:ILE:HG23	1:A:230:LEU:HD23	1.73	0.69
1:B:29:LEU:CD2	1:B:45:VAL:HG22	2.24	0.68
1:B:286:LEU:HB2	1:B:300:LYS:HA	1.78	0.66
1:B:319:ARG:HG2	2:B:409:HOH:O	1.95	0.66
1:B:24:LEU:HD23	1:B:24:LEU:N	2.12	0.65
1:B:220:THR:CG2	1:B:222:PHE:H	1.96	0.65
1:B:184:GLN:O	1:B:184:GLN:HG2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD22	1:A:239:LEU:HB3	1.77	0.64
1:B:47:ASP:OD1	1:B:51:ARG:HB2	1.97	0.64
1:A:30[A]:ARG:HG2	1:A:30[A]:ARG:HH11	1.62	0.64
1:B:162:ARG:HG2	1:B:162:ARG:NH1	2.11	0.64
1:B:188:ASN:OD1	1:B:190:ASN:HB2	1.97	0.63
1:A:220:THR:CG2	1:A:222:PHE:HB2	2.28	0.63
1:A:231:GLY:O	1:A:232:LYS:C	2.41	0.63
1:A:1:MET:CE	1:A:153:ASP:HB2	2.28	0.63
1:B:162:ARG:HA	1:B:331:TYR:O	1.99	0.63
1:A:48:ARG:NH1	1:A:263:ALA:O	2.30	0.62
1:A:161:TYR:O	1:A:332:ASP:HA	2.00	0.62
1:B:275:GLN:HE21	1:B:275:GLN:HA	1.65	0.62
1:A:184:GLN:OE1	1:A:293:LYS:HE2	2.00	0.61
1:B:6:ARG:O	1:B:6:ARG:HG2	1.97	0.61
1:B:46:LYS:HA	1:B:51:ARG:O	2.00	0.61
1:A:73:GLY:HA2	1:A:177:SER:CA	2.31	0.61
1:A:53:SER:HB2	1:A:267:ARG:HH22	1.63	0.60
1:A:57:LEU:HD23	1:A:57:LEU:N	2.16	0.60
1:B:101:LYS:HE3	1:B:101:LYS:O	2.02	0.60
1:A:28:LEU:O	1:A:29:LEU:HD23	2.01	0.60
1:A:62:LEU:O	1:A:63:GLU:C	2.45	0.59
1:B:88:PHE:HE2	1:B:97:LEU:HD21	1.67	0.59
1:B:27:ASP:OD1	1:B:28:LEU:HG	2.03	0.59
1:A:30[A]:ARG:HH11	1:A:30[A]:ARG:CG	2.15	0.59
1:A:57:LEU:HD13	1:A:298:TYR:CD2	2.38	0.59
1:B:29:LEU:HD21	1:B:45:VAL:HG22	1.86	0.58
1:A:310:ASN:ND2	1:A:323:VAL:HG13	2.20	0.57
1:B:262:HIS:CE1	1:B:264:ALA:HB3	2.40	0.57
1:A:1:MET:HE3	1:A:153:ASP:CB	2.34	0.57
1:B:220:THR:CG2	1:B:222:PHE:HD1	2.18	0.57
1:B:221:ALA:HB2	1:B:237:PHE:CD2	2.40	0.57
1:B:193:GLU:HA	1:B:228:VAL:O	2.04	0.57
1:A:1:MET:HE3	1:A:153:ASP:CG	2.31	0.56
1:B:32:ASP:HB2	1:B:41:THR:HG22	1.86	0.56
1:A:307:GLU:O	1:A:309:GLN:HG2	2.05	0.56
1:B:12:LEU:HB2	1:B:16:GLY:HA3	1.86	0.56
1:A:252:LYS:HD2	1:A:252:LYS:N	2.20	0.56
1:A:220:THR:CG2	1:A:222:PHE:HD1	2.18	0.56
1:B:125:ASN:OD1	1:B:125:ASN:N	2.39	0.55
1:B:197:GLU:HG3	2:B:452:HOH:O	2.07	0.55
1:A:23:GLN:OE1	1:A:30[B]:ARG:NE	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:THR:HG21	1:A:222:PHE:HB2	1.88	0.55
1:A:30[B]:ARG:HH11	1:A:30[B]:ARG:CG	2.20	0.54
1:A:299:PRO:O	1:A:300:LYS:C	2.47	0.54
1:B:262:HIS:O	1:B:266:GLY:N	2.39	0.54
1:B:59:PHE:HB2	1:B:65:TYR:CE1	2.42	0.54
1:B:73:GLY:HA2	1:B:177:SER:HA	1.89	0.54
1:B:182:ALA:HB2	1:B:262:HIS:NE2	2.21	0.54
1:B:220:THR:HG21	1:B:222:PHE:HB2	1.89	0.54
1:B:240:ASN:HD21	1:B:300:LYS:NZ	2.04	0.54
1:B:23:GLN:CD	1:B:30:ARG:HD2	2.32	0.53
1:A:101:LYS:O	1:A:102:GLU:C	2.51	0.53
1:B:32:ASP:C	1:B:33:ILE:HG13	2.32	0.53
1:A:221:ALA:HB2	1:A:237:PHE:CD2	2.44	0.53
1:B:220:THR:CG2	1:B:222:PHE:HB2	2.38	0.53
1:B:275:GLN:HE21	1:B:275:GLN:CA	2.19	0.53
1:B:58:GLY:C	1:B:293:LYS:HD3	2.34	0.53
1:B:89:LYS:HB3	1:B:93:LYS:O	2.09	0.53
1:B:63:GLU:CD	1:B:63:GLU:H	2.16	0.53
1:B:162:ARG:HH11	1:B:162:ARG:CG	2.20	0.52
1:A:203:PRO:HD2	1:A:213:GLU:O	2.10	0.52
1:B:145:LYS:O	1:B:163:ALA:HA	2.10	0.52
1:B:169:THR:OG1	1:B:170:PRO:HD2	2.09	0.52
1:B:197:GLU:HG2	1:B:249:LYS:NZ	2.25	0.52
1:B:220:THR:HG23	1:B:222:PHE:HD1	1.74	0.52
1:B:197:GLU:HG2	1:B:249:LYS:HZ2	1.75	0.52
1:A:184:GLN:OE1	1:A:293:LYS:HB2	2.09	0.52
1:B:265:SER:OG	1:B:267:ARG:HB2	2.10	0.52
1:A:182:ALA:HB2	1:A:262:HIS:CE1	2.46	0.51
1:A:162:ARG:HA	1:A:331:TYR:O	2.10	0.51
1:A:275:GLN:HE21	1:A:276:PRO:CD	2.21	0.51
1:A:4:VAL:HG11	1:A:122:VAL:HG13	1.92	0.51
1:B:275:GLN:HE21	1:B:276:PRO:HD2	1.74	0.51
1:A:23:GLN:HG3	1:A:30[B]:ARG:HD2	1.92	0.51
1:B:104:ASN:CG	1:B:209:ILE:HD11	2.36	0.51
1:A:319:ARG:HB2	2:A:461:HOH:O	2.10	0.51
1:B:9:PHE:CE2	1:B:62:LEU:HB2	2.45	0.51
1:B:162:ARG:NH1	1:B:330:GLU:OE2	2.44	0.51
1:A:199:ASP:O	1:A:217:VAL:HG22	2.11	0.50
1:A:182:ALA:HB2	1:A:262:HIS:NE2	2.27	0.50
1:B:219:GLY:N	2:B:417:HOH:O	2.36	0.50
1:B:11:GLU:OE2	1:B:18:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:HD2	1:B:72:PHE:CE1	2.47	0.50
1:B:254:LYS:HG3	1:B:336:TRP:CZ3	2.47	0.50
1:B:22:PHE:N	1:B:22:PHE:CD1	2.80	0.50
1:B:240:ASN:HD21	1:B:300:LYS:HZ3	1.58	0.50
1:B:275:GLN:HE21	1:B:276:PRO:CD	2.24	0.50
1:A:1:MET:HE3	1:A:153:ASP:HB2	1.91	0.49
1:A:136:GLY:O	1:A:137:GLU:C	2.52	0.49
1:A:186[A]:SER:OG	1:A:187:PRO:HD2	2.12	0.49
1:B:207:THR:O	1:B:208:LEU:HB2	2.12	0.49
1:B:254:LYS:HG3	1:B:336:TRP:CH2	2.47	0.49
1:B:23:GLN:C	1:B:24:LEU:HD23	2.37	0.49
1:A:111:ARG:HB3	2:A:452:HOH:O	2.12	0.49
1:A:57:LEU:HB2	1:A:72:PHE:CE2	2.47	0.49
1:A:284:ASN:OD1	1:A:301:HIS:HE1	1.95	0.49
1:A:70:PRO:HD2	1:A:72:PHE:CE1	2.48	0.49
1:B:203:PRO:HD2	1:B:213:GLU:O	2.13	0.49
1:A:311:TRP:CD1	1:A:311:TRP:N	2.80	0.49
1:A:62:LEU:O	1:A:65:TYR:N	2.41	0.49
1:B:311:TRP:CD1	1:B:311:TRP:N	2.80	0.49
1:A:167:GLN:O	1:A:168:ALA:C	2.56	0.48
1:B:300:LYS:HG3	1:B:301:HIS:ND1	2.28	0.48
1:B:165:ALA:HB2	1:B:325:LEU:HD23	1.95	0.48
1:A:104:ASN:HD21	1:A:207:THR:HB	1.79	0.48
1:B:79:VAL:HG11	1:B:83:ILE:HD11	1.95	0.48
1:B:82:ARG:HE	1:B:101:LYS:HZ3	1.60	0.48
1:B:299:PRO:HD2	1:B:302:SER:HB3	1.96	0.48
1:B:300:LYS:O	1:B:301:HIS:HB2	2.13	0.48
1:B:257:CYS:N	1:B:271:VAL:O	2.46	0.48
1:B:199:ASP:OD1	1:B:249:LYS:HE2	2.15	0.47
1:A:84:ALA:HA	1:A:209:ILE:CD1	2.43	0.47
1:B:170:PRO:HA	1:B:323:VAL:O	2.15	0.47
1:A:239:LEU:HA	1:A:239:LEU:HD23	1.43	0.47
1:A:49:GLN:HB2	1:A:51:ARG:HG3	1.96	0.46
1:B:158:ILE:HG12	1:B:336:TRP:CD1	2.50	0.46
1:A:73:GLY:CA	1:A:177:SER:HA	2.41	0.46
1:B:194:VAL:HG22	1:B:260:VAL:HG13	1.97	0.46
1:B:180:ASN:ND2	1:B:186:SER:HB2	2.30	0.46
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.51	0.46
1:B:288:GLY:HA2	1:B:298:TYR:O	2.16	0.46
1:A:188:ASN:HA	1:A:302:SER:HA	1.98	0.46
1:A:275:GLN:HE21	1:A:276:PRO:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TYR:HB2	1:A:336:TRP:HB2	1.97	0.46
1:B:299:PRO:HD2	1:B:302:SER:CB	2.46	0.46
1:A:30[B]:ARG:CG	1:A:30[B]:ARG:NH1	2.78	0.45
1:B:290:LEU:O	1:B:297:VAL:HA	2.16	0.45
1:B:288:GLY:HA2	1:B:298:TYR:C	2.40	0.45
1:A:30[B]:ARG:HH11	1:A:30[B]:ARG:HG3	1.80	0.45
1:B:310:ASN:ND2	1:B:323:VAL:HG13	2.30	0.45
1:B:292:GLY:HA3	1:B:298:TYR:CE1	2.52	0.45
1:B:318:PRO:HD2	2:B:409:HOH:O	2.17	0.45
1:B:278:VAL:O	1:B:278:VAL:HG13	2.16	0.45
1:B:208:LEU:N	1:B:208:LEU:HD23	2.32	0.45
1:A:57:LEU:HB2	1:A:72:PHE:HE2	1.82	0.45
1:A:292:GLY:HA3	1:A:298:TYR:CE1	2.52	0.45
1:B:262:HIS:ND1	1:B:265:SER:CB	2.80	0.45
1:B:310:ASN:ND2	1:B:323:VAL:CG1	2.80	0.45
1:B:31:VAL:HG22	1:B:43:LEU:HD13	1.99	0.45
1:A:118:TRP:HB3	1:A:129:PHE:HB3	1.99	0.45
1:B:82:ARG:HE	1:B:101:LYS:CE	2.29	0.44
1:B:297:VAL:CG1	1:B:298:TYR:N	2.80	0.44
1:A:292:GLY:N	1:A:296:ALA:O	2.48	0.44
1:B:44:GLU:HA	1:B:53:SER:O	2.17	0.44
1:B:294:ASN:C	1:B:296:ALA:H	2.25	0.44
1:A:200:THR:HB	1:A:214:VAL:HG12	1.99	0.44
1:B:220:THR:CG2	1:B:221:ALA:N	2.80	0.44
1:B:275:GLN:HA	1:B:275:GLN:NE2	2.32	0.44
1:B:291:LYS:H	1:B:291:LYS:HG3	1.46	0.44
1:A:180:ASN:ND2	1:A:189:ILE:CD1	2.80	0.44
1:A:265:SER:OG	1:A:267:ARG:HG3	2.17	0.44
1:B:82:ARG:HE	1:B:101:LYS:NZ	2.15	0.44
1:A:198:ALA:HA	1:A:249:LYS:HE2	2.00	0.44
1:A:257:CYS:HB3	1:A:271:VAL:O	2.18	0.44
1:A:200:THR:OG1	1:A:247:CYS:HB2	2.18	0.44
1:A:235:GLN:O	1:A:236:ASP:C	2.57	0.44
1:A:288:GLY:HA2	1:A:298:TYR:O	2.17	0.44
1:B:101:LYS:HE3	1:B:101:LYS:HB3	1.43	0.44
1:B:168:ALA:HA	1:B:325:LEU:O	2.18	0.44
1:B:9:PHE:CZ	1:B:62:LEU:N	2.86	0.43
1:B:297:VAL:HG12	1:B:298:TYR:N	2.33	0.43
1:B:102:GLU:HA	1:B:103:PRO:HA	1.72	0.43
1:A:115:LYS:C	1:A:116:VAL:HG13	2.43	0.43
1:B:189:ILE:HG12	1:B:301:HIS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:CD2	1:A:239:LEU:HB3	2.47	0.43
1:B:215:ALA:HA	1:B:216:PRO:HD3	1.96	0.43
1:A:220:THR:CG2	1:A:222:PHE:CD1	2.99	0.43
1:A:226:LYS:O	1:A:228:VAL:HG13	2.19	0.43
1:A:230:LEU:HA	1:A:230:LEU:HD12	1.59	0.43
1:B:48:ARG:NH2	1:B:263:ALA:O	2.51	0.43
1:B:300:LYS:CE	1:B:301:HIS:CE1	3.00	0.42
1:B:184:GLN:OE1	1:B:293:LYS:HE2	2.19	0.42
1:A:194:VAL:HG12	1:A:195:THR:N	2.34	0.42
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.89	0.42
1:B:231:GLY:O	1:B:232:LYS:C	2.60	0.42
1:B:9:PHE:CE2	1:B:62:LEU:CA	3.02	0.42
1:B:220:THR:CG2	1:B:222:PHE:CD1	3.01	0.42
1:A:30[A]:ARG:CG	1:A:30[A]:ARG:NH1	2.80	0.42
1:B:213:GLU:HB3	2:B:427:HOH:O	2.20	0.42
1:A:220:THR:HG22	1:A:222:PHE:HB2	1.98	0.42
1:B:2:ALA:HA	1:B:25:GLN:O	2.19	0.42
1:B:82:ARG:HE	1:B:101:LYS:HE2	1.85	0.42
1:A:209:ILE:O	1:A:210:PRO:C	2.63	0.42
1:A:290:LEU:O	1:A:297:VAL:HA	2.19	0.42
1:A:163:ALA:HB3	1:A:331:TYR:HB3	2.02	0.41
1:A:194:VAL:CG1	1:A:195:THR:N	2.82	0.41
1:A:252:LYS:N	1:A:252:LYS:CD	2.80	0.41
1:A:254:LYS:NZ	2:A:433:HOH:O	2.53	0.41
1:B:290:LEU:O	1:B:297:VAL:HG22	2.20	0.41
1:A:27:ASP:OD1	1:A:27:ASP:N	2.52	0.41
1:A:254:LYS:HG3	1:A:336:TRP:CZ3	2.56	0.41
1:A:170:PRO:C	1:A:171:VAL:HG23	2.45	0.41
1:B:261:HIS:CD2	1:B:268:VAL:HG22	2.55	0.41
1:B:286:LEU:O	1:B:300:LYS:HB2	2.21	0.41
1:A:251:SER:HB2	1:A:253:GLU:H	1.86	0.41
1:A:106:LEU:HG	1:A:107:HIS:N	2.36	0.41
1:A:278:VAL:HG13	1:A:278:VAL:O	2.19	0.41
1:B:9:PHE:HE2	1:B:62:LEU:HA	1.86	0.41
1:B:21:LYS:NZ	1:B:41:THR:HG21	2.36	0.41
1:B:290:LEU:HD23	1:B:290:LEU:HA	1.91	0.41
1:B:161:TYR:O	1:B:332:ASP:HA	2.20	0.41
1:A:114:ASP:OD1	1:A:114:ASP:N	2.54	0.40
1:A:30[A]:ARG:NH1	1:A:30[A]:ARG:HB3	2.36	0.40
1:A:257:CYS:N	1:A:271:VAL:O	2.50	0.40
1:B:186:SER:HA	1:B:187:PRO:HD3	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ALA:CA	1:A:209:ILE:CD1	2.99	0.40
1:B:180:ASN:HD21	1:B:186:SER:HB2	1.86	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	345/344 (100%)	315 (91%)	29 (8%)	1 (0%)	36	42
1	B	341/344 (99%)	318 (93%)	23 (7%)	0	100	100
All	All	686/688 (100%)	633 (92%)	52 (8%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLY

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	288/285 (101%)	258 (90%)	30 (10%)	7	7
1	B	285/285 (100%)	250 (88%)	35 (12%)	4	4
All	All	573/570 (100%)	508 (89%)	65 (11%)	6	5

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	THR
1	A	30[A]	ARG
1	A	30[B]	ARG
1	A	51	ARG
1	A	53	SER
1	A	55	VAL
1	A	57	LEU
1	A	67	GLN
1	A	68	LYS
1	A	76	ILE
1	A	83	ILE
1	A	89	LYS
1	A	106	LEU
1	A	189	ILE
1	A	209	ILE
1	A	220	THR
1	A	228	VAL
1	A	229	GLU
1	A	232	LYS
1	A	249	LYS
1	A	251	SER
1	A	252	LYS
1	A	254	LYS
1	A	275	GLN
1	A	291	LYS
1	A	297	VAL
1	A	317	GLN
1	A	323	VAL
1	A	338	LYS
1	B	5	THR
1	B	6	ARG
1	B	11	GLU
1	B	24	LEU
1	B	28	LEU
1	B	30	ARG
1	B	39	THR
1	B	41	THR
1	B	53	SER
1	B	55	VAL
1	B	75[A]	VAL
1	B	75[B]	VAL

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Mol	Chain	Res	Type
1	B	87	THR
1	B	89	LYS
1	B	93	LYS
1	B	101	LYS
1	B	115	LYS
1	B	121	ARG
1	B	162	ARG
1	B	184	GLN
1	B	186	SER
1	B	208	LEU
1	B	209	ILE
1	B	229	GLU
1	B	239	LEU
1	B	249	LYS
1	B	251	SER
1	B	252	LYS
1	B	254	LYS
1	B	275	GLN
1	B	291	LYS
1	B	300	LYS
1	B	315	VAL
1	B	329	GLU
1	B	341	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	67	GLN
1	A	96	HIS
1	A	128	GLN
1	A	240	ASN
1	A	275	GLN
1	A	301	HIS
1	B	67	GLN
1	B	235	GLN
1	B	238	HIS
1	B	240	ASN
1	B	275	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](#)

There are no ligands in this entry.

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	344/344 (100%)	-0.60	1 (0%) 90 88	21, 34, 60, 82	3 (0%)
1	B	342/344 (99%)	-0.50	0 100 100	19, 36, 65, 86	1 (0%)
All	All	686/688 (99%)	-0.55	1 (0%) 92 90	19, 35, 64, 86	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	GLY	2.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.