Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:13 PM GMT

PDB ID	:	1SNZ
Title	:	Crystal structure of apo human galactose mutarotase
Authors	:	Thoden, J.B.; Timson, D.J.; Reece, R.J.; Holden, H.M.
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

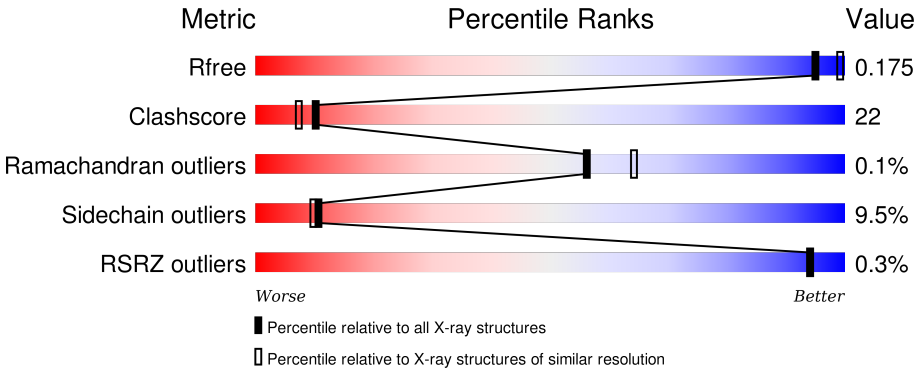
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	59% 33% 8% •
1	B	344	% 53% 37% 9% ••

2 Entry composition (i)

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.

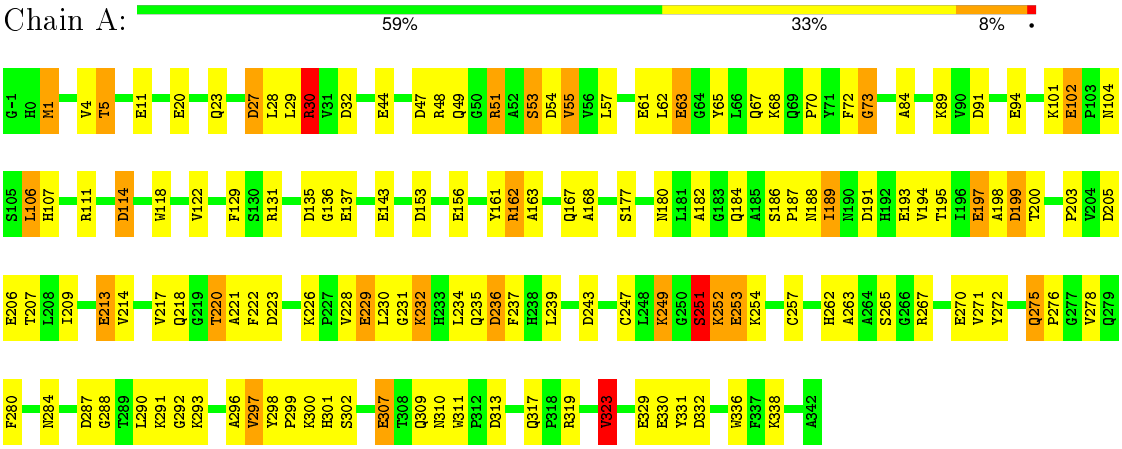
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	137	Total	O	0	0
			137	137		
2	B	121	Total	O	0	0
			121	121		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

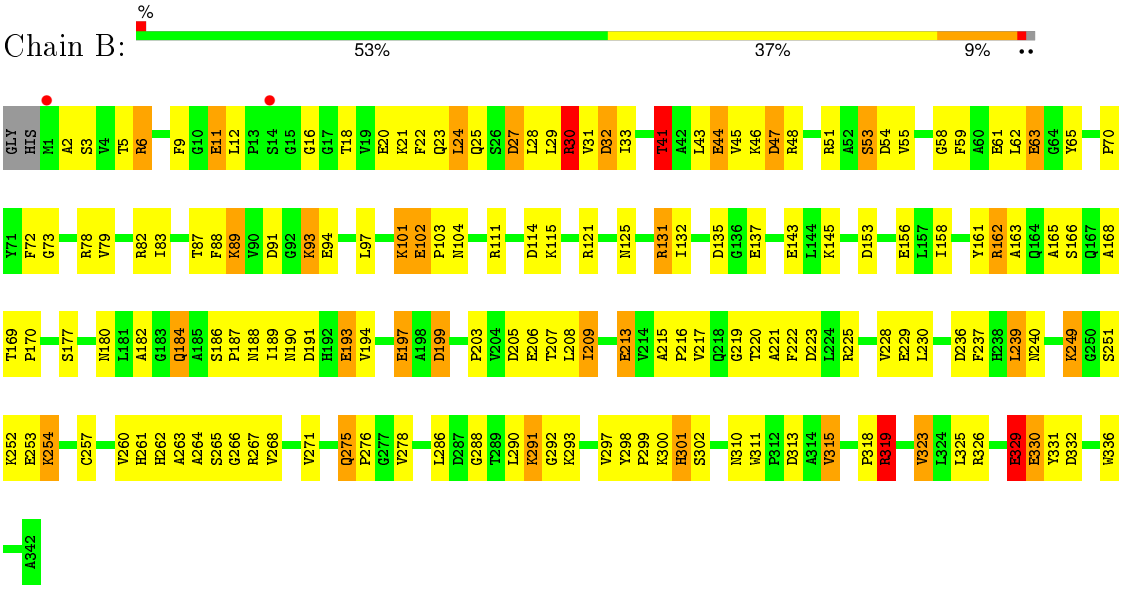
- Molecule 1: aldose 1-epimerase

Chain A:



- Molecule 1: aldose 1-epimerase

Chain B:



4 Data and refinement statistics (i)

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 45.35 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-2.20) 85.0 (45.35-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.56 (at 2.05Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.172 , 0.201 0.171 , 0.175	Depositor DCC
R_{free} test set	3713 reflections (11.80%)	DCC
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 84.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 43820 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.94	20/2788 (0.7%)	1.34	36/3787 (1.0%)
1	B	0.93	17/2752 (0.6%)	1.33	37/3740 (1.0%)
All	All	0.93	37/5540 (0.7%)	1.33	73/7527 (1.0%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	GLU	CD-OE2	7.24	1.33	1.25
1	B	253	GLU	CD-OE2	6.40	1.32	1.25
1	A	102	GLU	CD-OE2	6.36	1.32	1.25
1	B	102	GLU	CD-OE2	6.29	1.32	1.25
1	A	20	GLU	CD-OE2	6.20	1.32	1.25
1	B	197	GLU	CD-OE2	6.15	1.32	1.25
1	B	61	GLU	CD-OE2	6.08	1.32	1.25
1	B	143	GLU	CD-OE2	6.01	1.32	1.25
1	A	63	GLU	CD-OE2	6.00	1.32	1.25
1	B	44	GLU	CD-OE2	5.96	1.32	1.25
1	B	193	GLU	CD-OE2	5.96	1.32	1.25
1	A	206	GLU	CD-OE2	5.95	1.32	1.25
1	A	61	GLU	CD-OE2	5.92	1.32	1.25
1	A	143	GLU	CD-OE2	5.90	1.32	1.25
1	A	94	GLU	CD-OE2	5.87	1.32	1.25
1	B	213	GLU	CD-OE2	5.86	1.32	1.25
1	A	197	GLU	CD-OE2	5.83	1.32	1.25
1	A	330	GLU	CD-OE2	5.74	1.31	1.25
1	A	44	GLU	CD-OE2	5.73	1.31	1.25
1	A	156	GLU	CD-OE2	5.70	1.31	1.25
1	B	229	GLU	CD-OE2	5.70	1.31	1.25
1	B	330	GLU	CD-OE2	5.61	1.31	1.25
1	B	156	GLU	CD-OE2	5.59	1.31	1.25
1	B	94	GLU	CD-OE2	5.58	1.31	1.25
1	A	229	GLU	CD-OE2	5.57	1.31	1.25
1	B	63	GLU	CD-OE2	5.55	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	GLU	CD-OE2	5.47	1.31	1.25
1	B	20	GLU	CD-OE2	5.43	1.31	1.25
1	A	11	GLU	CD-OE2	5.37	1.31	1.25
1	A	270	GLU	CD-OE2	5.34	1.31	1.25
1	A	213	GLU	CD-OE2	5.30	1.31	1.25
1	A	329	GLU	CD-OE2	5.30	1.31	1.25
1	B	137	GLU	CD-OE2	5.27	1.31	1.25
1	A	307	GLU	CD-OE2	5.18	1.31	1.25
1	A	5	THR	CB-OG1	5.18	1.53	1.43
1	B	206	GLU	CD-OE2	5.11	1.31	1.25
1	A	193	GLU	CD-OE2	5.11	1.31	1.25

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	ASP	CB-CG-OD1	9.15	126.54	118.30
1	B	131	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	54	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	205	ASP	CB-CG-OD1	8.04	125.54	118.30
1	B	205	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	B	114	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	A	236	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	205	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	A	54	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	27	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	B	114	ASP	CB-CG-OD1	7.08	124.67	118.30
1	B	153	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	B	91	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	30[A]	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	30[B]	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	135	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	236	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	191	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	313	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	199	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	B	313	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	A	313	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	47	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	243	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	B	153	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	32	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	55	VAL	CG1-CB-CG2	6.32	121.02	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	78	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	54	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	236	ASP	CB-CG-OD1	6.22	123.89	118.30
1	B	135	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	251	SER	N-CA-C	-6.20	94.26	111.00
1	B	199	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	191	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	199	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	91	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	199	ASP	CB-CG-OD1	6.05	123.74	118.30
1	B	32	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	A	223	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	131	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	114	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	191	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	323	VAL	CB-CA-C	-5.90	100.19	111.40
1	A	32	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	41	THR	N-CA-CB	-5.83	99.23	110.30
1	B	30	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	287	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	220	THR	N-CA-CB	-5.68	99.50	110.30
1	B	313	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	54	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	47	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	111	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	47	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	280	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	A	287	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	27	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	111	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	223	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	319	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	243	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	236	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	323	VAL	CB-CA-C	-5.30	101.32	111.40
1	B	78	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	225	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	91	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	47	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	131	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	27	ASP	CB-CG-OD2	-5.14	113.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	315	VAL	CB-CA-C	-5.09	101.72	111.40
1	B	223	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	B	135	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	191	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2704	0	2629	104	0
1	B	2677	0	2605	126	0
2	A	137	0	0	3	0
2	B	121	0	0	5	0
All	All	5639	0	5234	230	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 (230) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:A:252:LYS:H	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:N	1:B:24:LEU:HD23	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
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:B:162:ARG:HG2	1:B:162:ARG:NH1	2.11	0.64
1:A:30[A]:ARG:HH11	1:A:30[A]:ARG:HG2	1.62	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: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:161:TYR:O	1:A:332:ASP:HA	2.00	0.62
1:A:48:ARG:NH1	1:A:263:ALA:O	2.30	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:46:LYS:HA	1:B:51:ARG:O	2.00	0.61
1:B:6:ARG:O	1:B:6:ARG:HG2	1.97	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:O	1:B:101:LYS:HE3	2.02	0.60
1:A:28:LEU:O	1:A:29:LEU:HD23	2.01	0.60
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:CG	1:A:30[A]:ARG:HH11	2.15	0.59
1:A:57:LEU:HD13	1:A:298:TYR:CD2	2.38	0.59
1:A:231:GLY:O	1:A:232:LYS:C	2.41	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:HIS:CE1	1:B:264:ALA:HB3	2.40	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: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:A:62:LEU:O	1:A:63:GLU:C	2.45	0.55
1:B:197:GLU:HG3	2:B:452:HOH:O	2.07	0.55
1:B:125:ASN:N	1:B:125:ASN:OD1	2.39	0.55
1:A:220:THR:HG21	1:A:222:PHE:HB2	1.88	0.55
1:A:23:GLN:OE1	1:A:30[B]:ARG:NE	2.40	0.55
1:B:262:HIS:O	1:B:266:GLY:N	2.39	0.54
1:A:30[B]:ARG:HH11	1:A:30[B]:ARG:CG	2.20	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:220:THR:CG2	1:B:222:PHE:HB2	2.38	0.53
1:A:221:ALA:HB2	1:A:237:PHE:CD2	2.44	0.53
1:B:275:GLN:HE21	1:B:275:GLN:CA	2.19	0.53
1:B:89:LYS:HB3	1:B:93:LYS:O	2.09	0.53
1:B:162:ARG:CG	1:B:162:ARG:HH11	2.20	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:NZ	2.25	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:A:203:PRO:HD2	1:A:213:GLU:O	2.10	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:B:275:GLN:HE21	1:B:276:PRO:HD2	1.74	0.51
1:A:4:VAL:HG11	1:A:122:VAL:HG13	1.92	0.51
1:A:23:GLN:HG3	1:A:30[B]:ARG:HD2	1.92	0.51
1:A:319:ARG:HB2	2:A:461:HOH:O	2.10	0.51
1:B:162:ARG:NH1	1:B:330:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PHE:CE2	1:B:62:LEU:HB2	2.45	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:70:PRO:HD2	1:B:72:PHE:CE1	2.47	0.50
1:B:11:GLU:OE2	1:B:18:THR:OG1	2.29	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:275:GLN:HE21	1:B:276:PRO:CD	2.24	0.50
1:A:299:PRO:O	1:A:300:LYS:C	2.47	0.49
1:B:254:LYS:HG3	1:B:336:TRP:CH2	2.47	0.49
1:B:207:THR:O	1:B:208:LEU:HB2	2.12	0.49
1:A:186[A]:SER:OG	1:A:187:PRO:HD2	2.12	0.49
1:B:23:GLN:CD	1:B:30:ARG:HD2	2.32	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:B:240:ASN:HD21	1:B:300:LYS:HZ3	1.59	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:32:ASP:C	1:B:33:ILE:HG13	2.32	0.49
1:B:311:TRP:N	1:B:311:TRP:CD1	2.80	0.49
1:A:101:LYS:O	1:A:102:GLU:C	2.51	0.48
1:B:300:LYS:HG3	1:B:301:HIS:ND1	2.28	0.48
1:B:58:GLY:C	1:B:293:LYS:HD3	2.34	0.48
1:B:165:ALA:HB2	1:B:325:LEU:HD23	1.95	0.48
1:B:79:VAL:HG11	1:B:83:ILE:HD11	1.95	0.48
1:A:104:ASN:HD21	1:A:207:THR:HB	1.79	0.48
1:B:63:GLU:CD	1:B:63:GLU:H	2.16	0.48
1:B:300:LYS:O	1:B:301:HIS:HB2	2.13	0.48
1:B:299:PRO:HD2	1:B:302:SER:HB3	1.96	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:1:MET:HE3	1:A:153:ASP:HB2	1.97	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:CG	1:B:209:ILE:HD11	2.36	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:A:136:GLY:O	1:A:137:GLU:C	2.52	0.46
1:B:180:ASN:ND2	1:B:186:SER:HB2	2.30	0.46
1:B:288:GLY:HA2	1:B:298:TYR:O	2.16	0.46
1:B:239:LEU:HA	1:B:239:LEU:HD23	1.51	0.46
1:A:275:GLN:HE21	1:A:276:PRO:HD2	1.80	0.46
1:A:188:ASN:HA	1:A:302:SER:HA	1.98	0.46
1:B:299:PRO:HD2	1:B:302:SER:CB	2.46	0.46
1:A:272:TYR:HB2	1:A:336:TRP:HB2	1.97	0.46
1:A:30[B]:ARG:NH1	1:A:30[B]:ARG:CG	2.78	0.45
1:B:290:LEU:O	1:B:297:VAL:HA	2.16	0.45
1:A:30[B]:ARG:HG3	1:A:30[B]:ARG:HH11	1.80	0.45
1:A:1:MET:HE1	1:A:153:ASP:OD1	2.17	0.45
1:B:310:ASN:ND2	1:B:323:VAL:HG13	2.30	0.45
1:B:318:PRO:HD2	2:B:409:HOH:O	2.17	0.45
1:B:292:GLY:HA3	1:B:298:TYR:CE1	2.52	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:B:262:HIS:ND1	1:B:265:SER:CB	2.80	0.45
1:A:292:GLY:HA3	1:A:298:TYR:CE1	2.52	0.45
1:A:57:LEU:HB2	1:A:72:PHE:HE2	1.82	0.45
1:A:1:MET:HE1	1:A:153:ASP:CG	2.38	0.45
1:B:82:ARG:HE	1:B:101:LYS:HZ3	1.63	0.45
1:B:310:ASN:ND2	1:B:323:VAL:CG1	2.80	0.45
1:B:23:GLN:C	1:B:24:LEU:HD23	2.37	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:B:44:GLU:HA	1:B:53:SER:O	2.17	0.44
1:A:292:GLY:N	1:A:296:ALA:O	2.48	0.44
1:B:220:THR:CG2	1:B:221:ALA:N	2.80	0.44
1:B:275:GLN:NE2	1:B:275:GLN:HA	2.32	0.44
1:A:200:THR:HB	1:A:214:VAL:HG12	1.99	0.44
1:B:291:LYS:HG3	1:B:291:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:GLN:O	1:A:168:ALA:C	2.56	0.44
1:A:288:GLY:HA2	1:A:298:TYR:O	2.17	0.44
1:B:101:LYS:HB3	1:B:101:LYS:HE3	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:B:189:ILE:HG12	1:B:301:HIS:O	2.17	0.43
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:HD12	1:A:230:LEU:HA	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:HA	1:B:230:LEU:HD12	1.89	0.42
1:B:220:THR:CG2	1:B:222:PHE:CD1	3.01	0.42
1:B:9:PHE:CE2	1:B:62:LEU:CA	3.02	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:82:ARG:HE	1:B:101:LYS:HE2	1.85	0.42
1:B:2:ALA:HA	1:B:25:GLN:O	2.19	0.42
1:A:290:LEU:O	1:A:297:VAL:HA	2.19	0.42
1:A:252:LYS:N	1:A:252:LYS:CD	2.80	0.41
1:A:163:ALA:HB3	1:A:331:TYR:HB3	2.02	0.41
1:A:254:LYS:NZ	2:A:433:HOH:O	2.53	0.41
1:A:194:VAL:CG1	1:A:195:THR:N	2.82	0.41
1:B:290:LEU:O	1:B:297:VAL:HG22	2.20	0.41
1:A:1:MET:CE	1:A:153:ASP:CB	2.96	0.41
1:A:254:LYS:HG3	1:A:336:TRP:CZ3	2.56	0.41
1:A:27:ASP:OD1	1:A:27:ASP:N	2.52	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:B:21:LYS:NZ	1:B:41:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PHE:HE2	1:B:62:LEU:HA	1.86	0.41
1:B:288:GLY:HA2	1:B:298:TYR:C	2.40	0.41
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.91	0.41
1:A:278:VAL:HG13	1:A:278:VAL:O	2.19	0.41
1:B:161:TYR:O	1:B:332:ASP:HA	2.20	0.41
1:A:114:ASP:N	1:A:114:ASP:OD1	2.54	0.40
1:A:30[A]:ARG:NH1	1:A:30[A]:ARG:HB3	2.36	0.40
1:B:186:SER:HA	1:B:187:PRO:HD3	1.82	0.40
1:A:257:CYS:N	1:A:271:VAL:O	2.50	0.40
1:A:235:GLN:O	1:A:236:ASP:C	2.57	0.40
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%)	46 50
1	B	341/344 (99%)	318 (93%)	23 (7%)	0	100 100
All	All	686/688 (100%)	633 (92%)	52 (8%)	1 (0%)	56 64

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%)	263 (91%)	25 (9%)	13 12
1	B	285/285 (100%)	255 (90%)	30 (10%)	8 8
All	All	573/570 (100%)	518 (90%)	55 (10%)	11 9

All (55) 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	67	GLN
1	A	68	LYS
1	A	89	LYS
1	A	106	LEU
1	A	162	ARG
1	A	189	ILE
1	A	218	GLN
1	A	229	GLU
1	A	232	LYS
1	A	249	LYS
1	A	251	SER
1	A	252	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	3	SER
1	B	5	THR

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Mol	Chain	Res	Type
1	B	6	ARG
1	B	11	GLU
1	B	24	LEU
1	B	30	ARG
1	B	41	THR
1	B	53	SER
1	B	55	VAL
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	166	SER
1	B	184	GLN
1	B	209	ILE
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	301	HIS
1	B	315	VAL
1	B	319	ARG
1	B	329	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	240	ASN
1	A	275	GLN
1	A	301	HIS
1	B	67	GLN
1	B	235	GLN
1	B	240	ASN
1	B	275	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.56	0 100 100	21, 34, 60, 82	0
1	B	342/344 (99%)	-0.48	2 (0%) 90 90	22, 36, 65, 86	0
All	All	686/688 (99%)	-0.52	2 (0%) 94 94	21, 35, 64, 86	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	2.5
1	B	14	SER	2.3

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.