Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 05:39 AM EDT

PDB ID	:	2HO5
Title	:	Crystal structure of Oxidoreductase, Gfo/Idh/MocA family from Streptococcus pneumoniae
Authors	:	Chang, C.; Hatzos, C.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2006-07-13
Resolution	:	2.56 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 (i) 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 (i)) were used in the production of this report:

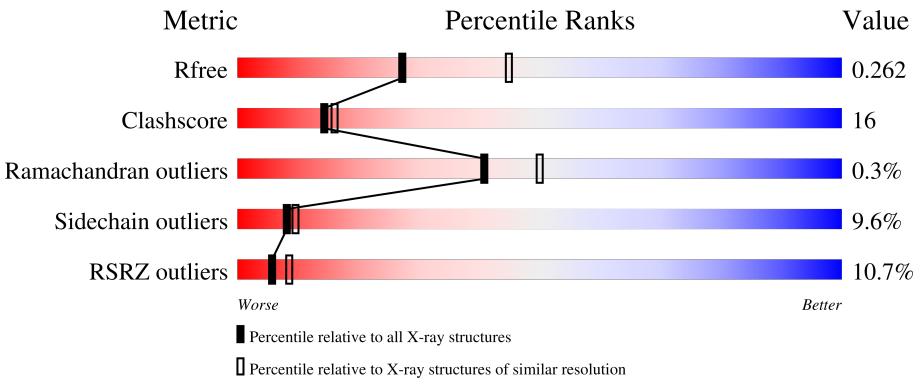
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.56 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 <=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	325	8% 67% 24% • 6%
1	B	325	12% 64% 24% 5% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4847 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 Oxidoreductase, Gfo/Idh/MocA family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	305	2413	1550	406	450	2	5	0	1	0
1	B	305	2421	1555	407	451	2	6	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
A	154	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
A	176	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
A	277	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
A	287	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
A	313	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
B	154	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
B	176	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
B	277	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
B	287	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8
B	313	MSE	MET	MODIFIED RESIDUE	UNP Q97PV8

- Molecule 2 is water.

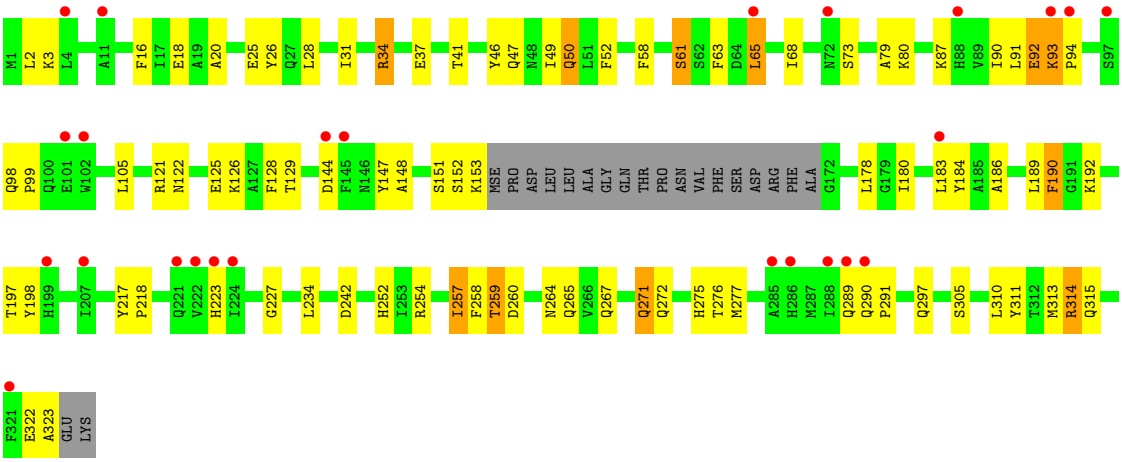
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	3	3	3	0	0
2	B	10	10	10	0	0

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.

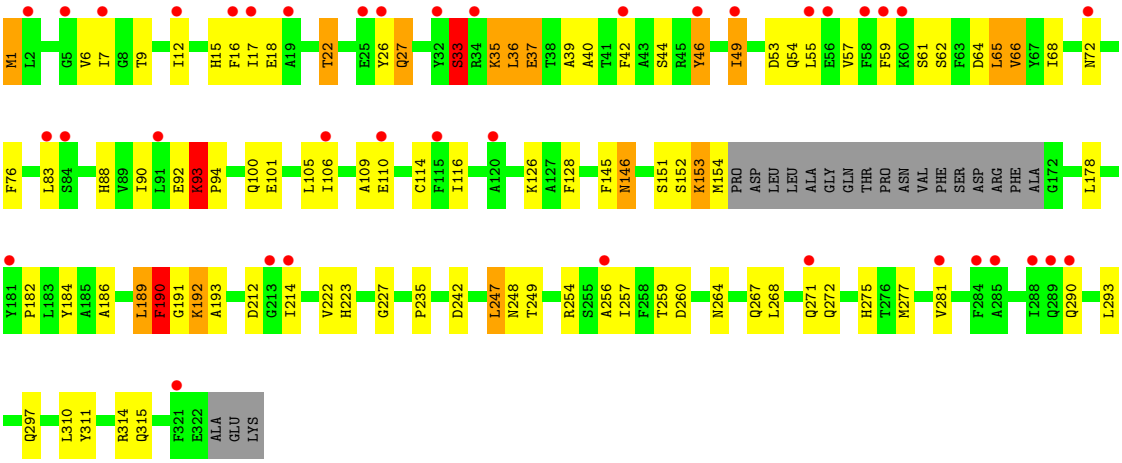
• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain A:



• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	117.11Å 117.11Å 102.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.56 41.41 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.56) 98.1 (41.41-2.56)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.88 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.266 0.208 , 0.262	Depositor DCC
R_{free} test set	1197 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	67.7	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4847	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2699e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.87	0/2471	0.86	1/3349 (0.0%)
1	B	1.01	7/2478 (0.3%)	0.87	3/3354 (0.1%)
All	All	0.94	7/4949 (0.1%)	0.86	4/6703 (0.1%)

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	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	LYS	CD-CE	17.22	1.94	1.51
1	B	37	GLU	CD-OE2	9.44	1.36	1.25
1	B	36	LEU	C-N	7.08	1.50	1.34
1	B	37	GLU	CD-OE1	6.90	1.33	1.25
1	B	33	SER	CB-OG	6.56	1.50	1.42
1	B	114	CYS	CB-SG	-6.37	1.71	1.82
1	B	36	LEU	C-O	5.30	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	242	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	189	LEU	O-C-N	-5.18	114.41	122.70
1	B	190	PHE	N-CA-C	5.08	124.70	111.00
1	A	314	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	GLU	Peptide

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	2413	0	2339	67	0
1	B	2421	0	2357	82	0
2	A	3	0	0	0	0
2	B	10	0	0	2	0
All	All	4847	0	4696	148	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 16.

All (148) 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:35:LYS:CD	1:B:35:LYS:CE	1.94	1.43
1:A:93:LYS:HB3	1:A:94:PRO:CD	1.67	1.23
1:B:93:LYS:HB3	1:B:94:PRO:HD2	1.17	1.10
1:B:93:LYS:HB3	1:B:94:PRO:CD	1.81	1.09
1:A:152:SER:HA	1:A:153:LYS:CB	1.87	1.04
1:A:93:LYS:HB3	1:A:94:PRO:HD2	1.05	1.03
1:B:93:LYS:CB	1:B:94:PRO:HD2	1.90	1.00
1:B:153:LYS:HA	1:B:154:MSE:HB2	1.46	0.98
1:A:16:PHE:HD1	1:A:277:MSE:CE	1.79	0.95
1:A:275:HIS:HD2	1:A:277:MSE:H	1.16	0.92
1:B:275:HIS:CD2	1:B:277:MSE:H	1.88	0.91
1:B:275:HIS:HD2	1:B:277:MSE:H	0.96	0.91
1:A:93:LYS:CB	1:A:94:PRO:CD	2.56	0.83
1:B:153:LYS:HA	1:B:154:MSE:CB	2.09	0.82
1:B:192:LYS:HZ2	1:B:192:LYS:HA	1.49	0.77
1:A:16:PHE:CD1	1:A:277:MSE:CE	2.70	0.72
1:B:72:ASN:HB2	1:B:93:LYS:NZ	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PHE:HD1	1:A:277:MSE:HE1	1.51	0.72
1:B:92:GLU:CG	1:B:93:LYS:H	2.04	0.71
1:B:6:VAL:HG21	1:B:17:ILE:HD11	1.71	0.71
1:B:93:LYS:CB	1:B:94:PRO:CD	2.52	0.71
1:A:46:TYR:HB2	1:A:49:ILE:HD13	1.74	0.68
1:A:16:PHE:CD1	1:A:277:MSE:HE1	2.28	0.67
1:B:44:SER:OG	2:B:326:HOH:O	2.13	0.67
1:A:192:LYS:HG3	1:A:305:SER:HB3	1.76	0.66
1:A:92:GLU:HG3	1:A:93:LYS:N	2.11	0.65
1:B:92:GLU:HG3	1:B:93:LYS:H	1.61	0.64
1:B:212:ASP:HB3	1:B:223:HIS:HE1	1.63	0.64
1:B:66:VAL:HG22	1:B:68:ILE:HG13	1.80	0.63
1:A:152:SER:CA	1:A:153:LYS:CB	2.71	0.63
1:B:33:SER:HB3	1:B:39:ALA:HB2	1.80	0.62
1:B:18:GLU:O	1:B:22:THR:OG1	2.16	0.62
1:A:260:ASP:OD2	1:A:264:ASN:HB2	2.00	0.61
1:B:275:HIS:HD2	1:B:277:MSE:N	1.81	0.61
1:B:72:ASN:HB2	1:B:93:LYS:HZ2	1.61	0.61
1:A:16:PHE:HD1	1:A:277:MSE:HE2	1.63	0.61
1:A:28:LEU:HD21	1:A:31:ILE:HD11	1.82	0.60
1:B:311:TYR:O	1:B:315:GLN:HG3	2.00	0.60
1:B:247:LEU:CD2	1:B:256:ALA:HB2	2.32	0.59
1:B:15[B]:HIS:CE1	1:B:275:HIS:CE1	2.91	0.59
1:B:7:ILE:HD12	1:B:68:ILE:HG12	1.85	0.59
1:A:31:ILE:HD12	1:A:49:ILE:HG21	1.85	0.59
1:A:257:ILE:HD11	1:A:265:GLN:HB3	1.84	0.59
1:B:65:LEU:HA	1:B:88:HIS:O	2.03	0.58
1:A:92:GLU:CG	1:A:93:LYS:N	2.66	0.58
1:B:247:LEU:HD23	1:B:256:ALA:CB	2.34	0.58
1:B:26:TYR:CE2	1:B:281:VAL:HG13	2.39	0.57
1:B:92:GLU:HG3	1:B:93:LYS:N	2.19	0.57
1:B:35:LYS:CE	1:B:35:LYS:CG	2.80	0.57
1:A:2:LEU:HB2	1:A:25:GLU:O	2.05	0.57
1:B:92:GLU:CG	1:B:93:LYS:N	2.68	0.57
1:B:192:LYS:NZ	1:B:193:ALA:H	2.01	0.57
1:A:257:ILE:CD1	1:A:265:GLN:HB3	2.34	0.56
1:B:268:LEU:N	1:B:268:LEU:HD12	2.20	0.56
1:A:198:TYR:HB2	1:A:313:MSE:HB3	1.88	0.56
1:B:1:MSE:HG2	1:B:27:GLN:HB2	1.86	0.56
1:A:275:HIS:CD2	1:A:277:MSE:H	2.08	0.56
1:A:275:HIS:HD2	1:A:277:MSE:N	1.96	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLN:HE21	1:A:271:GLN:HA	1.70	0.55
1:A:16:PHE:HB2	1:A:277:MSE:HE1	1.89	0.55
1:B:54:GLN:HA	1:B:54:GLN:OE1	2.06	0.55
1:B:105:LEU:HB3	1:B:116:ILE:HD13	1.87	0.55
1:A:310:LEU:O	1:A:314:ARG:HG3	2.07	0.55
1:A:50:GLN:HB2	1:A:52:PHE:HE1	1.72	0.55
1:B:106:ILE:O	1:B:110:GLU:HG3	2.08	0.54
1:B:26:TYR:HE2	1:B:281:VAL:HG13	1.73	0.54
1:B:186:ALA:O	1:B:189:LEU:O	2.26	0.53
1:B:247:LEU:HD23	1:B:256:ALA:HB2	1.89	0.53
1:A:98:GLN:HB2	1:A:99:PRO:CD	2.39	0.53
1:B:92:GLU:CD	1:B:93:LYS:H	2.12	0.52
1:B:46:TYR:HB2	1:B:49:ILE:HD11	1.91	0.52
1:A:186:ALA:O	1:A:189:LEU:O	2.28	0.51
1:B:76:PHE:CD1	1:B:101:GLU:HB3	2.45	0.51
1:A:65:LEU:HD21	1:A:90:ILE:HG13	1.92	0.51
1:B:310:LEU:O	1:B:314:ARG:HG3	2.11	0.50
1:A:16:PHE:CD1	1:A:277:MSE:HE2	2.42	0.50
1:A:68:ILE:HB	1:A:91:LEU:HD23	1.94	0.50
1:A:257:ILE:HD12	1:A:258:PHE:N	2.27	0.50
1:B:189:LEU:O	1:B:191:GLY:N	2.43	0.49
1:A:50:GLN:HB2	1:A:52:PHE:CE1	2.47	0.48
1:A:186:ALA:O	1:A:190:PHE:HB2	2.14	0.48
1:B:72:ASN:CB	1:B:93:LYS:NZ	2.75	0.48
1:A:58:PHE:O	1:A:61:SER:HB3	2.14	0.48
1:B:16:PHE:HD1	1:B:277:MSE:HE2	1.79	0.47
1:B:178:LEU:O	1:B:182:PRO:HD2	2.14	0.47
1:B:260:ASP:OD2	1:B:264:ASN:HB2	2.13	0.47
1:B:40:ALA:C	1:B:42:PHE:H	2.16	0.47
1:B:212:ASP:HB3	1:B:223:HIS:CE1	2.46	0.47
1:A:20:ALA:HB1	1:A:26:TYR:CG	2.50	0.47
1:A:242:ASP:OD1	1:A:242:ASP:N	2.47	0.47
1:B:83:LEU:HD22	1:B:109:ALA:HA	1.95	0.47
1:A:234:LEU:HD22	1:B:235:PRO:HD2	1.97	0.47
1:B:293:LEU:O	1:B:297:GLN:HG2	2.15	0.46
1:A:217:TYR:O	1:A:218:PRO:C	2.52	0.46
1:A:254:ARG:HG3	1:A:272:GLN:NE2	2.30	0.46
1:B:16:PHE:HD1	1:B:277:MSE:CE	2.27	0.46
1:B:62:SER:O	1:B:62:SER:OG	2.30	0.46
1:A:297:GLN:OE1	1:A:297:GLN:HA	2.15	0.46
1:B:268:LEU:N	1:B:268:LEU:CD1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HH11	1:A:34:ARG:HB3	1.80	0.45
1:B:254:ARG:HG3	1:B:272:GLN:NE2	2.32	0.45
1:A:16:PHE:CB	1:A:277:MSE:HE1	2.46	0.45
1:B:248:ASN:ND2	1:B:249:THR:HG23	2.32	0.45
1:A:98:GLN:HB2	1:A:99:PRO:HD2	1.98	0.45
1:B:40:ALA:HB3	2:B:331:HOH:O	2.15	0.45
1:B:214:ILE:HA	1:B:222:VAL:O	2.17	0.45
1:B:178:LEU:HD12	1:B:227:GLY:O	2.17	0.44
1:A:3:LYS:O	1:A:63:PHE:HB2	2.17	0.44
1:A:259:THR:HB	1:A:265:GLN:HG2	1.99	0.44
1:A:46:TYR:HB2	1:A:49:ILE:CD1	2.46	0.44
1:B:151:SER:OG	1:B:152:SER:N	2.51	0.44
1:A:148:ALA:HA	1:A:227:GLY:O	2.18	0.44
1:A:322:GLU:O	1:A:323:ALA:CB	2.66	0.43
1:B:36:LEU:O	1:B:39:ALA:N	2.50	0.43
1:A:144:ASP:OD2	1:A:223:HIS:HD2	2.01	0.43
1:B:27:GLN:HB2	1:B:27:GLN:HE21	1.70	0.43
1:B:153:LYS:HA	1:B:154:MSE:CG	2.47	0.43
1:B:153:LYS:CA	1:B:154:MSE:HB2	2.34	0.43
1:B:59:PHE:C	1:B:61:SER:H	2.21	0.43
1:B:145:PHE:HB3	1:B:182:PRO:HB3	2.01	0.43
1:A:121:ARG:HD2	1:A:276:THR:HB	2.00	0.43
1:B:72:ASN:H	1:B:93:LYS:HZ1	1.65	0.42
1:B:153:LYS:HA	1:B:154:MSE:HG2	2.01	0.42
1:B:65:LEU:HD23	1:B:90:ILE:HG13	2.00	0.42
1:B:190:PHE:CD1	1:B:190:PHE:N	2.86	0.42
1:B:93:LYS:HB2	1:B:94:PRO:HD2	1.93	0.42
1:B:128:PHE:HD1	1:B:189:LEU:HD21	1.83	0.42
1:A:190:PHE:N	1:A:190:PHE:CD1	2.88	0.42
1:B:146:ASN:ND2	1:B:146:ASN:C	2.73	0.42
1:A:128:PHE:O	1:A:129:THR:C	2.58	0.42
1:A:311:TYR:CE2	1:A:315:GLN:NE2	2.88	0.41
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.93	0.41
1:A:122:ASN:HA	1:A:125:GLU:OE2	2.20	0.41
1:A:271:GLN:HE21	1:A:271:GLN:CA	2.32	0.41
1:B:54:GLN:HB2	1:B:57:VAL:HB	2.01	0.41
1:B:247:LEU:CD2	1:B:256:ALA:CB	2.95	0.41
1:A:63:PHE:O	1:A:87:LYS:HD2	2.20	0.41
1:A:147:TYR:CE2	1:A:178:LEU:HD22	2.55	0.41
1:A:322:GLU:O	1:A:323:ALA:HB3	2.21	0.41
1:B:192:LYS:HZ2	1:B:192:LYS:CA	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:O	1:A:80:LYS:C	2.59	0.41
1:A:147:TYR:HD1	1:A:147:TYR:HA	1.77	0.41
1:A:311:TYR:O	1:A:315:GLN:HG3	2.21	0.41
1:B:192:LYS:HZ1	1:B:193:ALA:H	1.65	0.41
1:A:125:GLU:OE2	1:A:252:HIS:N	2.53	0.40
1:B:33:SER:O	1:B:53:ASP:HA	2.21	0.40
1:A:180:ILE:HA	1:A:183:LEU:HD12	2.04	0.40
1:B:15[B]:HIS:NE2	1:B:275:HIS:NE2	2.70	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	302/325 (93%)	287 (95%)	14 (5%)	1 (0%)	41	50
1	B	302/325 (93%)	283 (94%)	18 (6%)	1 (0%)	41	50
All	All	604/650 (93%)	570 (94%)	32 (5%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	LYS
1	B	93	LYS

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	250/263 (95%)	229 (92%)	21 (8%)	11 13
1	B	253/263 (96%)	226 (89%)	27 (11%)	6 7
All	All	503/526 (96%)	455 (90%)	48 (10%)	8 10

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	34	ARG
1	A	37	GLU
1	A	41	THR
1	A	47	GLN
1	A	50	GLN
1	A	61	SER
1	A	65	LEU
1	A	73	SER
1	A	126	LYS
1	A	151	SER
1	A	184	TYR
1	A	190	PHE
1	A	197	THR
1	A	257	ILE
1	A	259	THR
1	A	267	GLN
1	A	271	GLN
1	A	289	GLN
1	A	290	GLN
1	A	291	PRO
1	B	1	MSE
1	B	9	THR
1	B	12	ILE
1	B	22	THR
1	B	27	GLN
1	B	33	SER
1	B	37	GLU
1	B	46	TYR
1	B	49	ILE
1	B	55	LEU
1	B	64	ASP
1	B	65	LEU
1	B	66	VAL

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Mol	Chain	Res	Type
1	B	93	LYS
1	B	100	GLN
1	B	126	LYS
1	B	146	ASN
1	B	153	LYS
1	B	184	TYR
1	B	190	PHE
1	B	192	LYS
1	B	247	LEU
1	B	257	ILE
1	B	259	THR
1	B	267	GLN
1	B	271	GLN
1	B	290	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	146	ASN
1	A	194	ASN
1	A	202	GLN
1	A	223	HIS
1	A	271	GLN
1	A	275	HIS
1	B	27	GLN
1	B	124	HIS
1	B	146	ASN
1	B	223	HIS
1	B	252	HIS
1	B	272	GLN
1	B	275	HIS
1	B	315	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 monosaccharides 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	300/325 (92%)	0.62	25 (8%)	11	15	69, 80, 88, 96	0
1	B	299/325 (92%)	0.86	39 (13%)	3	4	45, 73, 83, 92	0
All	All	599/650 (92%)	0.74	64 (10%)	6	8	45, 77, 87, 96	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	TYR	6.7
1	B	46	TYR	5.9
1	B	17	ILE	5.9
1	B	288	ILE	5.4
1	B	281	VAL	5.2
1	B	284	PHE	5.0
1	B	42	PHE	4.8
1	B	12	ILE	4.8
1	B	91	LEU	4.8
1	B	289	GLN	4.7
1	B	55	LEU	4.6
1	B	72	ASN	4.4
1	B	60	LYS	4.1
1	B	2	LEU	4.1
1	A	93	LYS	4.0
1	A	97	SER	4.0
1	B	115	PHE	3.8
1	A	286	HIS	3.6
1	A	207	ILE	3.5
1	B	59	PHE	3.3
1	A	88	HIS	3.3
1	B	5	GLY	3.3
1	A	288	ILE	3.2
1	A	224	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	102	TRP	3.1
1	B	181	TYR	2.9
1	B	25	GLU	2.9
1	B	110	GLU	2.9
1	B	7	ILE	2.8
1	B	83	LEU	2.8
1	A	321	PHE	2.8
1	A	72	ASN	2.8
1	B	271	GLN	2.8
1	A	223	HIS	2.8
1	B	32	TYR	2.8
1	B	120	ALA	2.8
1	B	49	ILE	2.7
1	A	101	GLU	2.7
1	B	34	ARG	2.7
1	A	11	ALA	2.6
1	B	16	PHE	2.6
1	B	56	GLU	2.4
1	A	289	GLN	2.4
1	B	290	GLN	2.4
1	B	19	ALA	2.4
1	A	290	GLN	2.4
1	A	285	ALA	2.4
1	B	84	SER	2.4
1	A	65	LEU	2.4
1	A	144	ASP	2.4
1	A	221	GLN	2.3
1	B	285	ALA	2.3
1	B	214	ILE	2.3
1	A	183	LEU	2.3
1	A	94	PRO	2.3
1	B	321	PHE	2.2
1	A	4	LEU	2.2
1	B	256	ALA	2.2
1	B	213	GLY	2.1
1	B	106	ILE	2.1
1	A	145	PHE	2.1
1	A	199	HIS	2.1
1	A	222	VAL	2.1
1	B	58	PHE	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 monosaccharides 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.