



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:49 PM UTC

PDB ID : 3WTB / pdb_00003wtb
Title : Crystal structure of Gox0525
Authors : Yuan, Y.A.; Lin, J.P.
Deposited on : 2014-04-09
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
Xtrriage (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

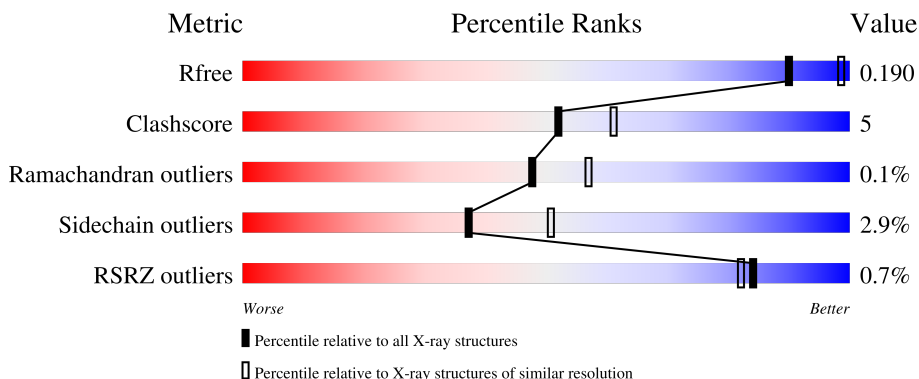
1 Overall quality at a glance i

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}	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	246	 90% 7% ..
1	B	246	 91% 8% ..
1	C	246	 90% 7% ...
1	D	246	 85% 12% ...
1	E	246	 87% 9% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	246	 <p>% 88% 9% ...</p>
1	G	246	 <p>84% 13% ..</p>
1	H	246	 <p>91% 6% ..</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14893 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	1773	1120	308	340	5	0	0	0
1	B	244	1773	1120	308	340	5	0	0	0
1	C	243	1763	1114	305	339	5	0	0	0
1	D	243	1763	1114	305	339	5	0	0	0
1	E	243	1763	1114	305	339	5	0	0	0
1	F	243	1763	1114	305	339	5	0	0	0
1	G	243	1763	1114	305	339	5	0	0	0
1	H	243	1763	1114	305	339	5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5FTJ3
A	-1	SER	-	expression tag	UNP Q5FTJ3
A	0	HIS	-	expression tag	UNP Q5FTJ3
B	-2	GLY	-	expression tag	UNP Q5FTJ3
B	-1	SER	-	expression tag	UNP Q5FTJ3
B	0	HIS	-	expression tag	UNP Q5FTJ3
C	-2	GLY	-	expression tag	UNP Q5FTJ3
C	-1	SER	-	expression tag	UNP Q5FTJ3
C	0	HIS	-	expression tag	UNP Q5FTJ3
D	-2	GLY	-	expression tag	UNP Q5FTJ3
D	-1	SER	-	expression tag	UNP Q5FTJ3
D	0	HIS	-	expression tag	UNP Q5FTJ3
E	-2	GLY	-	expression tag	UNP Q5FTJ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q5FTJ3
E	0	HIS	-	expression tag	UNP Q5FTJ3
F	-2	GLY	-	expression tag	UNP Q5FTJ3
F	-1	SER	-	expression tag	UNP Q5FTJ3
F	0	HIS	-	expression tag	UNP Q5FTJ3
G	-2	GLY	-	expression tag	UNP Q5FTJ3
G	-1	SER	-	expression tag	UNP Q5FTJ3
G	0	HIS	-	expression tag	UNP Q5FTJ3
H	-2	GLY	-	expression tag	UNP Q5FTJ3
H	-1	SER	-	expression tag	UNP Q5FTJ3
H	0	HIS	-	expression tag	UNP Q5FTJ3


- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	104	Total O 104 104	0	0
2	B	86	Total O 86 86	0	0
2	C	96	Total O 96 96	0	0
2	D	98	Total O 98 98	0	0
2	E	89	Total O 89 89	0	0
2	F	94	Total O 94 94	0	0
2	G	105	Total O 105 105	0	0
2	H	97	Total O 97 97	0	0

3 Residue-property plots [i](#)

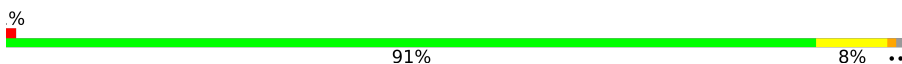
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative oxidoreductase

Chain A:  90% 7% ..




- Molecule 1: Putative oxidoreductase

Chain B:  91% 8% ..




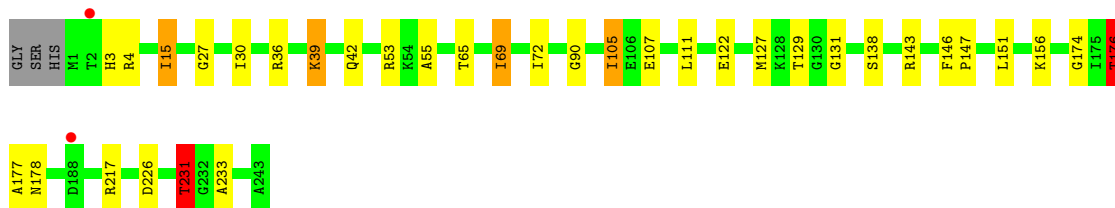
- Molecule 1: Putative oxidoreductase

Chain C:  90% 7% ...




- Molecule 1: Putative oxidoreductase

Chain D:  85% 12% ...



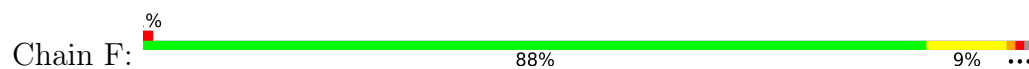
- Molecule 1: Putative oxidoreductase

Chain E:  87% 9% ..

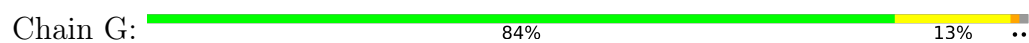




- Molecule 1: Putative oxidoreductase



- Molecule 1: Putative oxidoreductase



- Molecule 1: Putative oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	58.06Å 56.03Å 263.99Å 90.00° 93.20° 90.00°	Depositor
Resolution (Å)	49.73 – 2.20 49.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.73-2.20) 97.2 (49.73-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.155 , 0.186 0.161 , 0.190	Depositor DCC
R_{free} test set	4232 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14893	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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 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	1.12	0/1799	0.97	4/2442 (0.2%)
1	B	1.09	0/1799	0.98	3/2442 (0.1%)
1	C	1.09	1/1788 (0.1%)	1.00	5/2427 (0.2%)
1	D	1.09	0/1788	1.04	10/2427 (0.4%)
1	E	1.11	0/1788	1.07	7/2427 (0.3%)
1	F	1.17	2/1788 (0.1%)	1.06	9/2427 (0.4%)
1	G	1.17	2/1788 (0.1%)	1.07	7/2427 (0.3%)
1	H	1.06	0/1788	0.96	0/2427
All	All	1.11	5/14326 (0.0%)	1.02	45/19446 (0.2%)

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
1	F	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	188	ASP	CA-CB	5.59	1.62	1.53
1	F	150	SER	CB-OG	-5.50	1.31	1.42
1	G	228	SER	CB-OG	-5.27	1.31	1.42
1	F	228	SER	CB-OG	-5.26	1.31	1.42
1	C	192	GLU	N-CA	5.04	1.52	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	81	ARG	CB-CA-C	-10.69	90.23	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	108	VAL	CB-CA-C	-8.96	100.29	112.02
1	G	217	ARG	CB-CA-C	-8.61	96.50	110.79
1	G	108	VAL	CB-CA-C	-8.45	100.56	112.22
1	C	217	ARG	CB-CA-C	-7.76	97.91	110.79
1	E	217	ARG	CB-CA-C	-7.75	97.93	110.79
1	D	217	ARG	CB-CA-C	-7.73	97.95	110.79
1	F	217	ARG	CB-CA-C	-7.65	98.09	110.79
1	A	217	ARG	CB-CA-C	-7.49	98.36	110.79
1	D	176	THR	N-CA-CB	-7.47	98.89	110.85
1	G	150	SER	CB-CA-C	-7.46	98.88	110.81
1	F	150	SER	CB-CA-C	-7.45	98.88	110.81
1	D	231	THR	CA-CB-OG1	7.28	120.52	109.60
1	E	19	ILE	CA-CB-CG1	7.25	122.73	110.40
1	F	228	SER	CB-CA-C	-7.12	97.45	110.63
1	D	4	ARG	CG-CD-NE	7.09	127.59	112.00
1	B	1	MET	N-CA-C	6.63	122.78	113.56
1	B	36	ARG	N-CA-C	6.54	120.89	112.12
1	F	228	SER	N-CA-C	6.43	119.11	111.71
1	G	36	ARG	N-CA-C	-6.40	99.91	108.74
1	F	212	VAL	N-CA-CB	-6.39	102.48	110.47
1	G	190	ASN	CB-CA-C	6.28	121.51	111.15
1	G	228	SER	CB-CA-C	-6.09	97.47	110.32
1	C	179	VAL	CB-CA-C	-6.07	101.65	110.63
1	C	191	PRO	N-CA-C	6.06	121.51	113.57
1	D	231	THR	CB-CA-C	-6.00	97.81	109.68
1	D	105	ILE	CA-CB-CG1	5.85	120.35	110.40
1	E	108	VAL	N-CA-CB	5.82	118.02	110.57
1	D	217	ARG	CA-CB-CG	5.57	125.23	114.10
1	C	36	ARG	N-CA-C	-5.52	100.92	109.14
1	F	217	ARG	CA-CB-CG	5.51	125.11	114.10
1	E	23	LEU	CB-CG-CD2	5.47	127.10	110.70
1	E	23	LEU	CB-CG-CD1	-5.45	94.35	110.70
1	G	217	ARG	CA-CB-CG	5.44	124.99	114.10
1	A	36	ARG	N-CA-C	5.42	122.33	110.80
1	A	217	ARG	CA-CB-CG	5.30	124.70	114.10
1	F	150	SER	N-CA-CB	-5.28	102.07	109.94
1	D	39	LYS	CB-CG-CD	-5.18	99.39	111.30
1	B	217	ARG	N-CA-CB	5.13	118.24	110.28
1	D	231	THR	N-CA-CB	5.13	120.41	111.13
1	A	107	GLU	CB-CA-C	5.10	119.26	110.79
1	D	107	GLU	CB-CA-C	5.10	119.26	110.79
1	C	217	ARG	CA-CB-CG	5.09	124.28	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	192	GLU	CA-C-N	-5.05	113.51	122.20
1	F	192	GLU	C-N-CA	-5.05	113.51	122.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	242	VAL	Peptide
1	F	192	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	1773	0	1809	20	1
1	B	1773	0	1809	13	0
1	C	1763	0	1802	14	1
1	D	1763	0	1802	31	0
1	E	1763	0	1802	25	3
1	F	1763	0	1802	19	4
1	G	1763	0	1802	28	0
1	H	1763	0	1802	10	0
2	A	104	0	0	3	0
2	B	86	0	0	3	0
2	C	96	0	0	1	0
2	D	98	0	0	10	0
2	E	89	0	0	6	2
2	F	94	0	0	6	0
2	G	105	0	0	5	0
2	H	97	0	0	2	0
All	All	14893	0	14430	145	6

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 5.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HH21	1:G:143:ARG:NH2	1.20	1.40
1:D:143:ARG:HH21	1:E:143:ARG:NH2	1.13	1.40
1:A:143:ARG:NH2	1:G:143:ARG:HH21	1.18	1.39
1:D:143:ARG:NH2	1:E:143:ARG:HH21	1.15	1.35
1:A:143:ARG:NH2	1:G:143:ARG:NH2	1.72	1.32
1:D:143:ARG:NH2	1:E:143:ARG:NH2	1.68	1.31
1:D:111:LEU:HB3	2:D:392:HOH:O	1.30	1.28
1:G:99:GLN:HG2	2:G:330:HOH:O	1.52	1.10
1:E:23:LEU:CG	2:E:373:HOH:O	1.99	1.10
1:E:23:LEU:HG	2:E:373:HOH:O	1.50	1.04
1:B:33:THR:HG21	2:B:372:HOH:O	1.66	0.96
1:H:33:THR:HG21	2:H:368:HOH:O	1.67	0.95
1:D:176:THR:HG21	2:D:303:HOH:O	1.75	0.86
1:E:36:ARG:NH1	2:E:386:HOH:O	2.10	0.83
1:G:190:ASN:HB3	2:G:352:HOH:O	1.81	0.81
1:D:231:THR:HG21	2:D:309:HOH:O	1.79	0.79
1:D:143:ARG:HH21	1:E:143:ARG:HH22	1.31	0.79
1:G:76:HIS:HD2	2:G:378:HOH:O	1.65	0.79
1:G:33:THR:HG21	2:G:370:HOH:O	1.82	0.77
1:E:23:LEU:CD1	2:E:373:HOH:O	2.28	0.76
1:E:19:ILE:O	1:E:23:LEU:HD13	1.86	0.76
1:F:18:ALA:CB	1:F:212:VAL:HG13	2.16	0.75
1:E:187:THR:HG22	1:E:189:LEU:H	1.52	0.75
1:E:53:ARG:NH1	2:E:360:HOH:O	2.21	0.74
1:B:10:GLY:H	1:B:33:THR:HG22	1.50	0.74
1:G:187:THR:HG22	1:G:189:LEU:H	1.52	0.73
1:G:10:GLY:H	1:G:33:THR:HG22	1.55	0.71
1:H:10:GLY:H	1:H:33:THR:HG22	1.55	0.71
1:G:143:ARG:HD2	2:G:345:HOH:O	1.91	0.70
1:F:99:GLN:HG3	2:F:336:HOH:O	1.91	0.70
1:A:211:LYS:HE3	2:A:358:HOH:O	1.91	0.69
1:G:189:LEU:O	1:G:190:ASN:OD1	2.11	0.68
1:A:143:ARG:HH21	1:G:143:ARG:HH22	1.37	0.67
1:A:237:VAL:HG13	1:C:230:ILE:HD13	1.76	0.66
1:A:237:VAL:HG13	1:C:230:ILE:CD1	2.25	0.66
1:F:18:ALA:CB	1:F:212:VAL:CG1	2.73	0.66
1:D:42:GLN:HG2	2:D:384:HOH:O	1.97	0.65
1:F:18:ALA:HB2	1:F:212:VAL:CG1	2.25	0.65
1:H:100:MET:SD	1:H:151:LEU:HD22	2.37	0.65
1:E:127:MET:HE3	1:E:131:GLY:HA3	1.78	0.64
1:G:127:MET:HE3	1:G:131:GLY:HA3	1.78	0.64
1:H:22:LYS:HE2	2:H:345:HOH:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:MET:HE3	1:D:131:GLY:HA3	1.81	0.62
1:A:127:MET:HE3	1:A:131:GLY:HA3	1.80	0.61
1:F:192:GLU:OE2	2:F:357:HOH:O	2.16	0.61
1:B:127:MET:HE3	1:B:131:GLY:HA3	1.83	0.60
1:F:13:ARG:HD2	2:F:392:HOH:O	2.02	0.60
1:C:192:GLU:OE2	2:C:390:HOH:O	2.17	0.59
1:F:127:MET:HE3	1:F:131:GLY:HA3	1.83	0.59
1:E:104:GLN:O	1:E:108:VAL:HG23	2.03	0.58
1:G:104:GLN:O	1:G:108:VAL:HG23	2.03	0.58
1:F:187:THR:HG22	1:F:212:VAL:HG23	1.84	0.58
1:A:72:ILE:HG13	1:A:122:GLU:HB3	1.86	0.58
1:E:187:THR:HG22	1:E:189:LEU:N	2.19	0.57
1:E:22:LYS:NZ	1:E:213:ASN:HD21	2.02	0.57
1:A:192:GLU:O	1:A:201:ARG:NH2	2.38	0.57
1:F:18:ALA:HB2	1:F:212:VAL:HG11	1.86	0.57
1:G:72:ILE:HG13	1:G:122:GLU:HB3	1.87	0.57
1:G:196:ALA:O	1:G:199:VAL:HG22	2.05	0.57
1:F:12:SER:HB3	2:F:356:HOH:O	2.05	0.56
1:D:72:ILE:HG13	1:D:122:GLU:HB3	1.87	0.56
1:A:15:ILE:HG13	2:A:334:HOH:O	2.05	0.55
1:C:191:PRO:O	1:C:192:GLU:CB	2.52	0.55
1:B:243:ALA:HB3	2:B:349:HOH:O	2.05	0.55
1:C:163:THR:OG1	1:C:179:VAL:HG22	2.06	0.55
1:C:72:ILE:HG13	1:C:122:GLU:HB3	1.89	0.55
1:G:22:LYS:NZ	1:G:213:ASN:HD21	2.06	0.54
1:F:22:LYS:NZ	1:F:213:ASN:HD21	2.05	0.54
1:H:72:ILE:HG13	1:H:122:GLU:HB3	1.88	0.54
1:F:72:ILE:HG13	1:F:122:GLU:HB3	1.89	0.54
1:B:72:ILE:HG13	1:B:122:GLU:HB3	1.88	0.54
1:G:13:ARG:HE	1:G:189:LEU:HD21	1.74	0.53
1:E:72:ILE:HG13	1:E:122:GLU:HB3	1.89	0.53
1:A:237:VAL:HG22	1:C:230:ILE:HD12	1.90	0.53
1:D:176:THR:HG22	2:D:307:HOH:O	2.08	0.53
1:G:187:THR:HG22	1:G:189:LEU:N	2.20	0.52
1:F:42:GLN:NE2	2:F:367:HOH:O	2.41	0.52
1:A:53:ARG:NH2	1:D:226:ASP:OD1	2.43	0.52
1:D:176:THR:HA	1:D:231:THR:HG23	1.93	0.51
1:D:143:ARG:CZ	1:E:143:ARG:NH2	2.64	0.50
1:H:65:THR:O	1:H:69:ILE:HG13	2.13	0.49
1:B:178:ASN:HD22	1:B:233:ALA:H	1.61	0.49
1:G:178:ASN:HD22	1:G:233:ALA:H	1.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:THR:O	1:G:69:ILE:HG13	2.13	0.48
1:D:65:THR:O	1:D:69:ILE:HG13	2.14	0.48
1:D:36:ARG:NE	2:D:301:HOH:O	2.47	0.48
1:F:65:THR:O	1:F:69:ILE:HG13	2.14	0.48
1:C:178:ASN:HD22	1:C:233:ALA:H	1.62	0.47
1:D:105:ILE:HD13	1:D:151:LEU:HD11	1.96	0.47
1:B:53:ARG:HE	1:B:53:ARG:HA	1.78	0.47
1:D:129:THR:HG23	1:D:174:GLY:HA3	1.97	0.47
1:F:12:SER:CB	2:F:356:HOH:O	2.63	0.47
1:D:178:ASN:HD22	1:D:233:ALA:H	1.62	0.46
1:B:53:ARG:HA	1:B:53:ARG:NE	2.30	0.46
1:C:65:THR:O	1:C:69:ILE:HG13	2.15	0.46
1:E:65:THR:O	1:E:69:ILE:HG13	2.15	0.46
1:B:33:THR:CG2	2:B:372:HOH:O	2.42	0.45
1:D:143:ARG:HD2	2:D:320:HOH:O	2.15	0.45
1:B:65:THR:O	1:B:69:ILE:HG13	2.16	0.45
1:H:129:THR:HG23	1:H:174:GLY:HA3	1.99	0.45
1:A:65:THR:O	1:A:69:ILE:HG13	2.17	0.44
1:C:30:ILE:O	1:C:55:ALA:HA	2.18	0.44
1:D:177:ALA:H	1:D:231:THR:CG2	2.29	0.44
1:H:38:GLU:HG2	1:H:42:GLN:HE21	1.82	0.44
1:D:176:THR:CG2	2:D:307:HOH:O	2.66	0.44
1:E:30:ILE:O	1:E:55:ALA:HA	2.17	0.44
1:B:30:ILE:O	1:B:55:ALA:HA	2.18	0.44
1:C:178:ASN:ND2	1:C:233:ALA:H	2.16	0.43
1:D:178:ASN:ND2	1:D:233:ALA:H	2.16	0.43
1:G:14:GLY:HA2	1:G:187:THR:HG23	1.99	0.43
1:H:30:ILE:O	1:H:55:ALA:HA	2.19	0.43
1:E:23:LEU:HD12	1:E:23:LEU:N	2.33	0.43
1:G:178:ASN:ND2	1:G:233:ALA:H	2.16	0.43
1:D:30:ILE:O	1:D:55:ALA:HA	2.19	0.43
1:C:163:THR:HG21	1:C:179:VAL:HG23	2.01	0.43
1:F:178:ASN:HD22	1:F:233:ALA:H	1.65	0.43
1:D:39:LYS:HB3	1:D:39:LYS:HE2	1.58	0.43
1:D:90:GLY:HA2	2:D:392:HOH:O	2.19	0.43
1:C:138:SER:HB3	1:C:156:LYS:HG3	2.00	0.42
1:E:138:SER:HB3	1:E:156:LYS:HG3	2.01	0.42
1:F:30:ILE:O	1:F:55:ALA:HA	2.19	0.42
1:G:30:ILE:O	1:G:55:ALA:HA	2.20	0.42
1:D:105:ILE:HD13	1:D:151:LEU:CD1	2.50	0.42
1:A:129:THR:HG23	1:A:174:GLY:HA3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:THR:HA	1:B:33:THR:HB	2.02	0.42
1:A:53:ARG:NH1	2:A:320:HOH:O	2.43	0.42
1:E:23:LEU:HD12	2:E:373:HOH:O	2.08	0.42
1:G:138:SER:HB3	1:G:156:LYS:HG3	2.02	0.42
1:D:3:HIS:HD2	1:D:27:GLY:O	2.02	0.41
1:G:13:ARG:HE	1:G:189:LEU:CD2	2.33	0.41
1:E:129:THR:HG23	1:E:174:GLY:HA3	2.02	0.41
1:B:178:ASN:ND2	1:B:233:ALA:H	2.18	0.41
1:A:143:ARG:CZ	1:G:143:ARG:HH21	2.12	0.41
1:F:7:LEU:CD2	1:F:72:ILE:HD13	2.51	0.41
1:H:178:ASN:ND2	1:H:233:ALA:H	2.19	0.41
1:D:146:PHE:HB2	1:D:147:PRO:HD2	2.03	0.41
1:E:15:ILE:O	1:E:19:ILE:HG12	2.21	0.41
1:F:178:ASN:ND2	1:F:233:ALA:H	2.19	0.41
1:A:143:ARG:CZ	1:G:143:ARG:NH2	2.67	0.40
1:D:15:ILE:HG13	2:D:325:HOH:O	2.20	0.40
1:D:138:SER:HB3	1:D:156:LYS:HG3	2.02	0.40
1:A:5:VAL:HG21	1:A:79:PHE:HB3	2.04	0.40
1:A:30:ILE:O	1:A:55:ALA:HA	2.21	0.40
1:C:91:ILE:HG23	1:C:111:LEU:HD23	2.04	0.40
1:E:140:PHE:HA	1:E:143:ARG:O	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ARG:CZ	1:F:193:ASP:OD1[1_565]	1.88	0.32
1:E:13:ARG:NH2	1:F:193:ASP:OD1[1_565]	2.00	0.20
1:A:36:ARG:NH2	1:C:193:ASP:OD1[1_655]	2.08	0.12
1:E:13:ARG:NH1	1:F:193:ASP:OD1[1_565]	2.14	0.06
1:F:193:ASP:OD2	2:E:386:HOH:O[1_545]	2.19	0.01
2:E:387:HOH:O	2:E:387:HOH:O[2_756]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	242/246 (98%)	237 (98%)	5 (2%)	0	100	100
1	B	242/246 (98%)	238 (98%)	4 (2%)	0	100	100
1	C	241/246 (98%)	236 (98%)	4 (2%)	1 (0%)	30	34
1	D	241/246 (98%)	238 (99%)	3 (1%)	0	100	100
1	E	241/246 (98%)	238 (99%)	3 (1%)	0	100	100
1	F	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
1	G	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
1	H	241/246 (98%)	238 (99%)	3 (1%)	0	100	100
All	All	1930/1968 (98%)	1897 (98%)	32 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	GLU

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	176/177 (99%)	171 (97%)	5 (3%)	38	52
1	B	176/177 (99%)	172 (98%)	4 (2%)	44	59
1	C	175/177 (99%)	172 (98%)	3 (2%)	53	69
1	D	175/177 (99%)	170 (97%)	5 (3%)	37	51
1	E	175/177 (99%)	168 (96%)	7 (4%)	28	38
1	F	175/177 (99%)	171 (98%)	4 (2%)	44	59
1	G	175/177 (99%)	168 (96%)	7 (4%)	28	38
1	H	175/177 (99%)	169 (97%)	6 (3%)	32	44
All	All	1402/1416 (99%)	1361 (97%)	41 (3%)	37	51

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	53	ARG
1	A	69	ILE
1	A	192	GLU
1	A	211	LYS
1	B	15	ILE
1	B	33	THR
1	B	69	ILE
1	B	143	ARG
1	C	15	ILE
1	C	69	ILE
1	C	179	VAL
1	D	15	ILE
1	D	53	ARG
1	D	69	ILE
1	D	176	THR
1	D	231	THR
1	E	15	ILE
1	E	36	ARG
1	E	69	ILE
1	E	108	VAL
1	E	111	LEU
1	E	187	THR
1	E	202	LYS
1	F	15	ILE
1	F	69	ILE
1	F	150	SER
1	F	212	VAL
1	G	15	ILE
1	G	33	THR
1	G	53	ARG
1	G	64	SER
1	G	69	ILE
1	G	108	VAL
1	G	202	LYS
1	H	15	ILE
1	H	22	LYS
1	H	33	THR
1	H	69	ILE
1	H	151	LEU
1	H	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	68	ASN
1	A	178	ASN
1	B	59	GLN
1	B	68	ASN
1	B	173	GLN
1	B	178	ASN
1	C	68	ASN
1	C	178	ASN
1	D	3	HIS
1	D	25	GLN
1	D	68	ASN
1	D	178	ASN
1	E	68	ASN
1	E	173	GLN
1	E	178	ASN
1	E	213	ASN
1	F	59	GLN
1	F	68	ASN
1	F	178	ASN
1	F	213	ASN
1	G	68	ASN
1	G	178	ASN
1	G	213	ASN
1	H	42	GLN
1	H	68	ASN
1	H	178	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](#)

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

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	244/246 (99%)	-0.43	1 (0%) 88 87	19, 26, 47, 79	0
1	B	244/246 (99%)	-0.40	3 (1%) 76 74	18, 27, 49, 110	0
1	C	243/246 (98%)	-0.41	1 (0%) 88 87	19, 27, 50, 83	0
1	D	243/246 (98%)	-0.39	2 (0%) 82 80	18, 26, 53, 97	0
1	E	243/246 (98%)	-0.40	2 (0%) 82 80	18, 28, 49, 103	0
1	F	243/246 (98%)	-0.41	3 (1%) 76 74	18, 27, 51, 72	0
1	G	243/246 (98%)	-0.43	0 100 100	19, 26, 49, 70	0
1	H	243/246 (98%)	-0.43	1 (0%) 88 87	19, 28, 46, 80	0
All	All	1946/1968 (98%)	-0.41	13 (0%) 84 82	18, 27, 50, 110	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	LEU	4.3
1	E	1	MET	3.2
1	C	189	LEU	3.1
1	A	189	LEU	2.7
1	B	243	ALA	2.6
1	E	2	THR	2.6
1	H	1	MET	2.5
1	F	189	LEU	2.5
1	F	188	ASP	2.3
1	D	188	ASP	2.3
1	F	193	ASP	2.2
1	B	188	ASP	2.2
1	D	2	THR	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.