Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 PM GMT

PDB ID	:	3WTB
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
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:

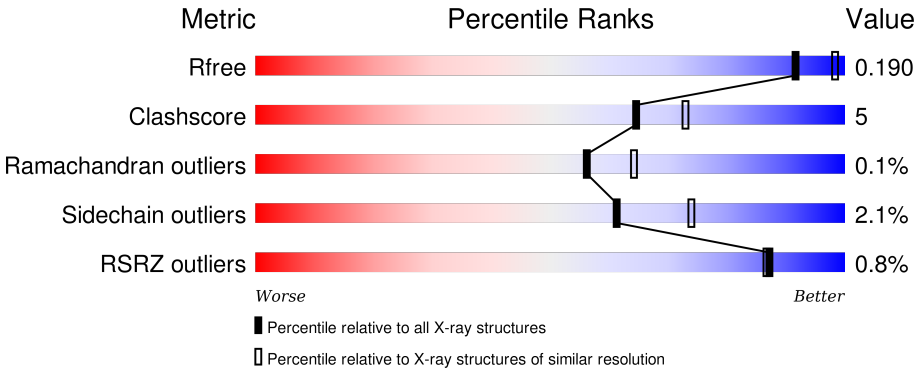
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	246	91% 7%
1	B	246	2% 91% 6%
1	C	246	89% 9%
1	D	246	% 85% 13%
1	E	246	% 87% 9%

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Mol	Chain	Length	Quality of chain
1	F	246	
1	G	246	
1	H	246	

2 Entry composition

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
1	A	244	Total	C	N	O	S	0	0	0
			1773	1120	308	340	5			
1	B	244	Total	C	N	O	S	0	0	0
			1773	1120	308	340	5			
1	C	243	Total	C	N	O	S	0	0	0
			1763	1114	305	339	5			
1	D	243	Total	C	N	O	S	0	0	0
			1763	1114	305	339	5			
1	E	243	Total	C	N	O	S	0	0	0
			1763	1114	305	339	5			
1	F	243	Total	C	N	O	S	0	0	0
			1763	1114	305	339	5			
1	G	243	Total	C	N	O	S	0	0	0
			1763	1114	305	339	5			
1	H	243	Total	C	N	O	S	0	0	0
			1763	1114	305	339	5			

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

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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.

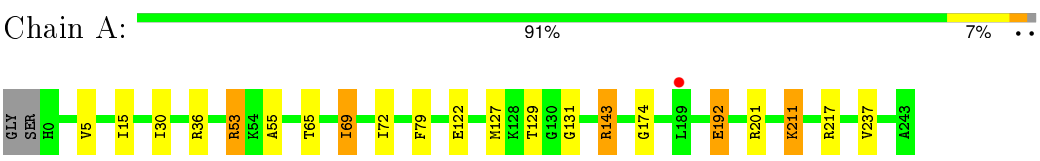
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	104	Total O 104 104	0	0
2	B	86	Total O 86 86	0	0
2	C	96	Total O 96 96	0	0
2	D	98	Total O 98 98	0	0
2	E	89	Total O 89 89	0	0
2	F	94	Total O 94 94	0	0
2	G	105	Total O 105 105	0	0
2	H	97	Total O 97 97	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

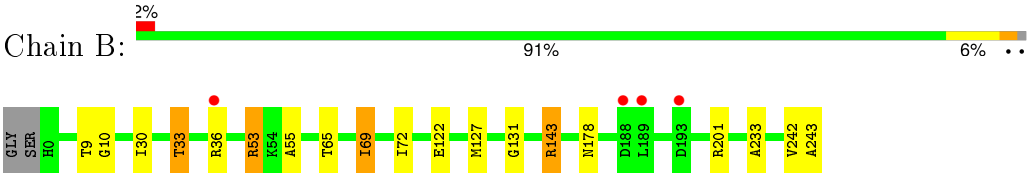
- Molecule 1: Putative oxidoreductase

Chain A:



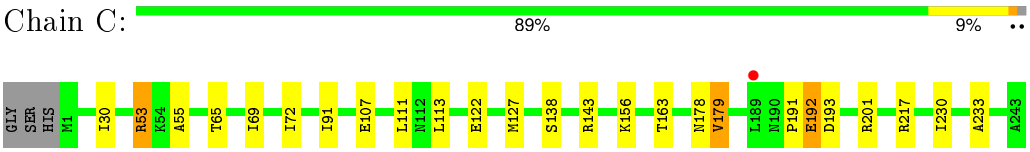
- Molecule 1: Putative oxidoreductase

Chain B:



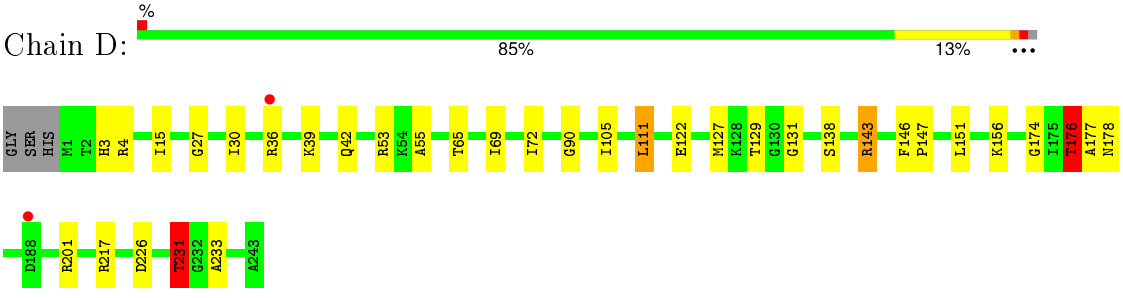
- Molecule 1: Putative oxidoreductase

Chain C:



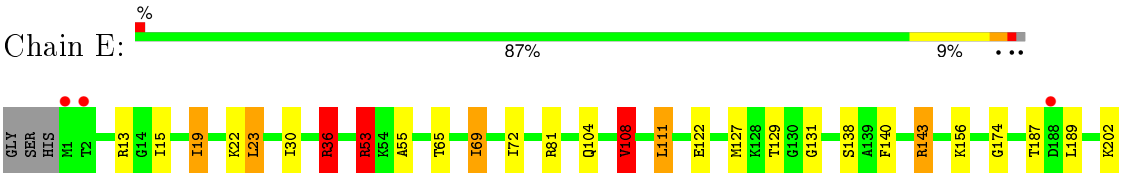
- Molecule 1: Putative oxidoreductase

Chain D:



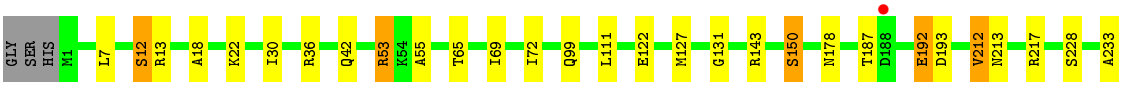
- Molecule 1: Putative oxidoreductase

Chain E:



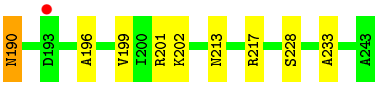
• Molecule 1: Putative oxidoreductase

Chain F:



• Molecule 1: Putative oxidoreductase

Chain G:



• Molecule 1: Putative oxidoreductase

Chain H:

4 Data and refinement statistics (i)

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 47.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.73-2.20) 97.1 (47.24-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.155 , 0.186 0.161 , 0.190	Depositor DCC
R_{free} test set	4229 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 84573 reflections (0.002%)	Xtriage
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

Xtriage'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.*

[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	0.82	0/1799	0.85	4/2442 (0.2%)
1	B	0.82	0/1799	0.88	7/2442 (0.3%)
1	C	0.82	1/1788 (0.1%)	0.92	10/2427 (0.4%)
1	D	0.81	0/1788	0.95	13/2427 (0.5%)
1	E	0.81	0/1788	1.01	14/2427 (0.6%)
1	F	0.90	3/1788 (0.2%)	0.94	12/2427 (0.5%)
1	G	0.88	2/1788 (0.1%)	0.95	13/2427 (0.5%)
1	H	0.78	1/1788 (0.1%)	0.88	8/2427 (0.3%)
All	All	0.83	7/14326 (0.0%)	0.92	81/19446 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	150	SER	CB-OG	-8.53	1.31	1.42
1	G	228	SER	CB-OG	-8.18	1.31	1.42
1	F	228	SER	CB-OG	-8.17	1.31	1.42
1	C	107	GLU	CD-OE2	6.58	1.32	1.25
1	F	12	SER	CB-OG	-6.43	1.33	1.42
1	G	64	SER	CB-OG	-5.76	1.34	1.42
1	H	12	SER	CB-OG	-5.38	1.35	1.42

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	143	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	E	143	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	G	143	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	143	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	E	53	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	E	81	ARG	CB-CA-C	-10.09	90.23	110.40
1	E	23	LEU	CB-CG-CD1	-9.79	94.35	111.00
1	F	53	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	E	23	LEU	CB-CG-CD2	9.47	127.10	111.00
1	F	143	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	C	143	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	H	143	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	C	53	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	D	4	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	H	13	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	C	201	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	53	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	143	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	F	53	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	201	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	4	ARG	CG-CD-NE	7.52	127.59	111.80
1	B	201	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	36	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	H	151	LEU	CA-CB-CG	7.09	131.60	115.30
1	E	36	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	E	111	LEU	CA-CB-CG	6.95	131.29	115.30
1	G	217	ARG	CB-CA-C	-6.95	96.50	110.40
1	D	111	LEU	CB-CG-CD1	6.83	122.62	111.00
1	H	13	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	53	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	201	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	F	228	SER	CB-CA-C	-6.66	97.45	110.10
1	G	228	SER	CB-CA-C	-6.65	97.47	110.10
1	C	53	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	F	111	LEU	CB-CG-CD1	6.57	122.16	111.00
1	G	13	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	E	53	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	G	201	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	G	143	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	C	217	ARG	CB-CA-C	-6.24	97.91	110.40
1	E	217	ARG	CB-CA-C	-6.24	97.93	110.40
1	D	217	ARG	CB-CA-C	-6.22	97.95	110.40
1	E	143	ARG	NE-CZ-NH2	-6.21	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	19	ILE	CA-CB-CG1	6.18	122.73	111.00
1	F	217	ARG	CB-CA-C	-6.16	98.09	110.40
1	A	217	ARG	CB-CA-C	-6.02	98.36	110.40
1	D	176	THR	N-CA-CB	-6.00	98.89	110.30
1	H	36	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	G	111	LEU	CB-CG-CD1	5.94	121.09	111.00
1	G	150	SER	CB-CA-C	-5.91	98.88	110.10
1	F	150	SER	CB-CA-C	-5.90	98.88	110.10
1	H	143	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	E	108	VAL	CB-CA-C	-5.85	100.29	111.40
1	E	23	LEU	CA-CB-CG	5.78	128.60	115.30
1	H	151	LEU	CB-CG-CD2	5.77	120.81	111.00
1	G	108	VAL	CB-CA-C	-5.70	100.56	111.40
1	D	4	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	F	150	SER	N-CA-CB	-5.62	102.07	110.50
1	C	127	MET	CA-CB-CG	5.59	122.81	113.30
1	G	190	ASN	CB-CA-C	5.55	121.51	110.40
1	G	13	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	F	143	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	F	36	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	231	THR	CA-CB-OG1	5.49	120.52	109.00
1	B	36	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	143	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	217	ARG	CA-CB-CG	5.38	125.23	113.40
1	E	111	LEU	CB-CG-CD1	5.37	120.12	111.00
1	F	234	SER	CB-CA-C	-5.35	99.93	110.10
1	F	217	ARG	CA-CB-CG	5.33	125.11	113.40
1	D	231	THR	N-CA-CB	5.32	120.41	110.30
1	C	143	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	G	217	ARG	CA-CB-CG	5.27	124.99	113.40
1	A	143	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	113	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	201	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	217	ARG	CA-CB-CG	5.14	124.70	113.40
1	C	179	VAL	CB-CA-C	-5.13	101.65	111.40
1	H	127	MET	CA-CB-CG	5.12	122.00	113.30
1	D	231	THR	CB-CA-C	-5.11	97.81	111.60
1	G	13	ARG	CG-CD-NE	5.05	122.40	111.80

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:10:GLY:H	1:H:33:THR:HG22	1.55	0.71
1:G:10:GLY:H	1:G: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:F:18:ALA:HB2	1:F:212:VAL:CG1	2.25	0.65
1:D:42:GLN:HG2	2:D:384:HOH:O	1.97	0.65
1:H:100:MET:SD	1:H:151:LEU:HD22	2.37	0.65
1:H:22:LYS:HE2	2:H:345:HOH:O	1.97	0.64
1:F:192:GLU:OE2	2:F:357:HOH:O	2.16	0.61
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:A:127:MET:HE3	1:A:131:GLY:HA3	1.84	0.59
1:E:127:MET:HE3	1:E:131:GLY:HA3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:18:ALA:HB2	1:F:212:VAL:HG11	1.86	0.57
1:A:192:GLU:O	1:A:201:ARG:NH2	2.38	0.57
1:G:196:ALA:O	1:G:199:VAL:HG22	2.05	0.57
1:G:72:ILE:HG13	1:G:122:GLU:HB3	1.87	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:D:127:MET:HE3	1:D:131:GLY:HA3	1.88	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:G:127:MET:HE3	1:G:131:GLY:HA3	1.88	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:F:127:MET:HE3	1:F:131:GLY:HA3	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:B:127:MET:HE3	1:B:131:GLY:HA3	1.90	0.53
1:E:72:ILE:HG13	1:E:122:GLU:HB3	1.89	0.53
1:D:176:THR:HG22	2:D:307:HOH:O	2.08	0.53
1:A:237:VAL:HG22	1:C:230:ILE:HD12	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ILE:HD13	1:D:151:LEU:HD11	1.96	0.47
1:F:12:SER:CB	2:F:356:HOH:O	2.63	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: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:N	1:E:23:LEU:HD12	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:90:GLY:HA2	2:D:392:HOH:O	2.19	0.43
1:D:39:LYS:HB3	1:D:39:LYS:HE2	1.58	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
1:B:9:THR:HA	1:B:33:THR:HB	2.02	0.42
1:E:23:LEU:HD12	2:E:373:HOH:O	2.08	0.42
1:A:53:ARG:NH1	2:A:320:HOH:O	2.43	0.42
1:G:138:SER:HB3	1:G:156:LYS:HG3	2.02	0.42
1:G:13:ARG:HE	1:G:189:LEU:CD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:HIS:HD2	1:D:27:GLY:O	2.02	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: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:D:146:PHE:HB2	1:D:147:PRO:HD2	2.03	0.41
1:A:143:ARG:CZ	1:G:143:ARG:NH2	2.67	0.40
1:D:138:SER:HB3	1:D:156:LYS:HG3	2.02	0.40
1:D:15:ILE:HG13	2:D:325:HOH:O	2.20	0.40
1:E:140:PHE:HA	1:E:143:ARG:O	2.21	0.40
1:C:91:ILE:HG23	1:C:111:LEU:HD23	2.04	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

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 (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	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%)	39	42
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%)	56	64

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%)	172 (98%)	4 (2%)	58	71
1	B	176/177 (99%)	173 (98%)	3 (2%)	68	81
1	C	175/177 (99%)	174 (99%)	1 (1%)	90	95
1	D	175/177 (99%)	172 (98%)	3 (2%)	68	81
1	E	175/177 (99%)	169 (97%)	6 (3%)	44	54
1	F	175/177 (99%)	172 (98%)	3 (2%)	68	81
1	G	175/177 (99%)	169 (97%)	6 (3%)	44	54
1	H	175/177 (99%)	171 (98%)	4 (2%)	58	71
All	All	1402/1416 (99%)	1372 (98%)	30 (2%)	61	74

All (30) residues with a non-rotameric sidechain are listed below:

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	178	ASN
1	B	59	GLN
1	B	68	ASN
1	B	99	GLN
1	B	178	ASN
1	C	68	ASN
1	C	178	ASN
1	D	3	HIS

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Mol	Chain	Res	Type
1	D	25	GLN
1	D	68	ASN
1	D	178	ASN
1	E	68	ASN
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

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	244/246 (99%)	-0.52	1 (0%)	93	93	19, 26, 47, 79	0
1	B	244/246 (99%)	-0.52	4 (1%)	74	73	18, 27, 49, 110	0
1	C	243/246 (98%)	-0.54	1 (0%)	93	93	19, 27, 50, 83	0
1	D	243/246 (98%)	-0.50	2 (0%)	87	87	18, 26, 53, 97	0
1	E	243/246 (98%)	-0.52	3 (1%)	81	80	18, 28, 49, 103	0
1	F	243/246 (98%)	-0.56	1 (0%)	93	93	18, 27, 51, 72	0
1	G	243/246 (98%)	-0.55	3 (1%)	81	80	19, 26, 49, 70	0
1	H	243/246 (98%)	-0.54	1 (0%)	93	93	19, 28, 46, 80	0
All	All	1946/1968 (98%)	-0.53	16 (0%)	87	87	18, 27, 50, 110	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	5.6
1	B	189	LEU	4.9
1	B	188	ASP	3.9
1	G	36	ARG	3.1
1	D	188	ASP	2.9
1	E	2	THR	2.8
1	H	1	MET	2.6
1	G	193	ASP	2.6
1	E	188	ASP	2.5
1	A	189	LEU	2.3
1	D	36	ARG	2.3
1	B	193	ASP	2.3
1	B	36	ARG	2.3
1	F	188	ASP	2.2
1	C	189	LEU	2.1
1	G	42	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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.