Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 12:59 AM EST

PDB ID	:	4O9T
Title	:	Mechanism of transhydrogenase coupling proton translocation and hydride transfer
Authors	:	Leung, J.H.; Yamaguchi, M.; Moeller, A.; Schurig-Briccio, L.A.; Gennis, R.B.; Potter, C.S.; Carragher, B.; Stout, C.D.
Deposited on	:	2014-01-02
Resolution	:	3.08 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:

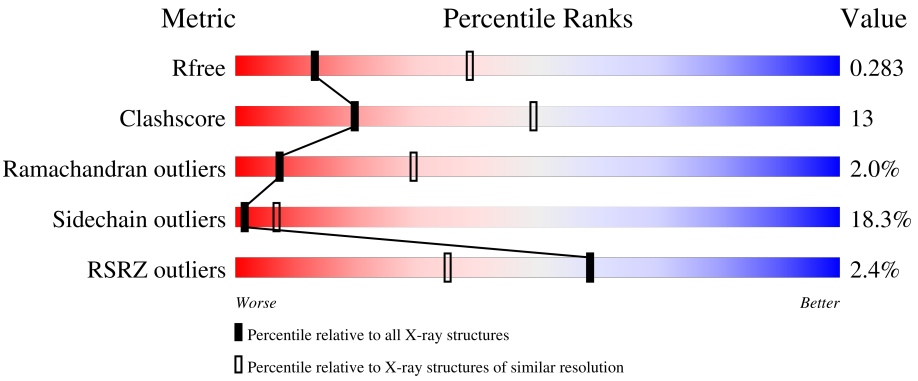
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	100	61% 26% 6% • 6%
1	C	100	3% 57% 24% 8% 11%
1	E	100	2% 58% 28% 6% • 6%
1	G	100	5% 55% 27% 6% • 11%
2	B	283	% 62% 24% 6% 7%

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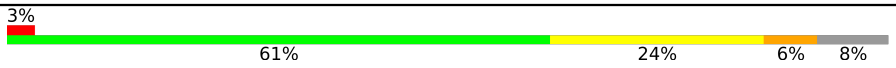
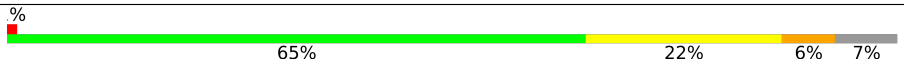
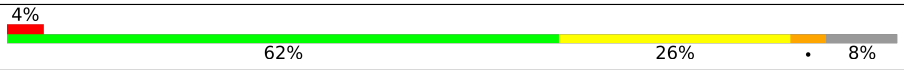
Mol	Chain	Length	Quality of chain
2	D	283	
2	F	283	
2	H	283	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10352 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 NAD(P) transhydrogenase subunit alpha 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			713	475	114	119	5			
1	C	89	Total	C	N	O	S	0	0	0
			666	444	105	112	5			
1	E	94	Total	C	N	O	S	0	0	0
			713	475	114	119	5			
1	G	89	Total	C	N	O	S	0	0	0
			666	444	105	112	5			

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			1904	1269	304	315	16			
2	D	260	Total	C	N	O	S	0	0	0
			1893	1262	302	313	16			
2	F	262	Total	C	N	O	S	0	0	0
			1904	1269	304	315	16			
2	H	260	Total	C	N	O	S	0	0	0
			1893	1262	302	313	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	276	HIS	-	expression tag	UNP Q72GS0
B	277	HIS	-	expression tag	UNP Q72GS0
B	278	HIS	-	expression tag	UNP Q72GS0
B	279	HIS	-	expression tag	UNP Q72GS0
B	280	HIS	-	expression tag	UNP Q72GS0
B	281	HIS	-	expression tag	UNP Q72GS0
B	282	HIS	-	expression tag	UNP Q72GS0
B	283	HIS	-	expression tag	UNP Q72GS0

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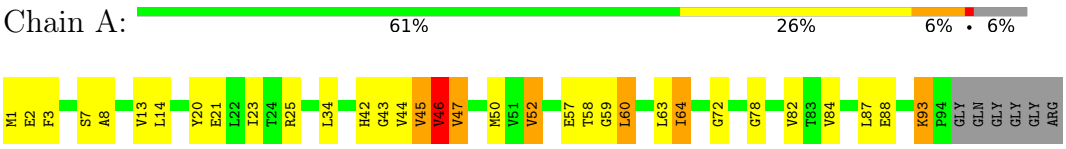
Chain	Residue	Modelled	Actual	Comment	Reference
D	276	HIS	-	expression tag	UNP Q72GS0
D	277	HIS	-	expression tag	UNP Q72GS0
D	278	HIS	-	expression tag	UNP Q72GS0
D	279	HIS	-	expression tag	UNP Q72GS0
D	280	HIS	-	expression tag	UNP Q72GS0
D	281	HIS	-	expression tag	UNP Q72GS0
D	282	HIS	-	expression tag	UNP Q72GS0
D	283	HIS	-	expression tag	UNP Q72GS0
F	276	HIS	-	expression tag	UNP Q72GS0
F	277	HIS	-	expression tag	UNP Q72GS0
F	278	HIS	-	expression tag	UNP Q72GS0
F	279	HIS	-	expression tag	UNP Q72GS0
F	280	HIS	-	expression tag	UNP Q72GS0
F	281	HIS	-	expression tag	UNP Q72GS0
F	282	HIS	-	expression tag	UNP Q72GS0
F	283	HIS	-	expression tag	UNP Q72GS0
H	276	HIS	-	expression tag	UNP Q72GS0
H	277	HIS	-	expression tag	UNP Q72GS0
H	278	HIS	-	expression tag	UNP Q72GS0
H	279	HIS	-	expression tag	UNP Q72GS0
H	280	HIS	-	expression tag	UNP Q72GS0
H	281	HIS	-	expression tag	UNP Q72GS0
H	282	HIS	-	expression tag	UNP Q72GS0
H	283	HIS	-	expression tag	UNP Q72GS0

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.

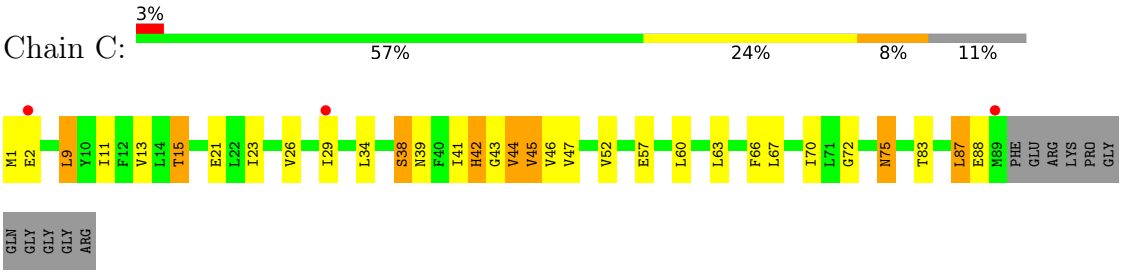
• Molecule 1: NAD(P) transhydrogenase subunit alpha 2

Chain A:



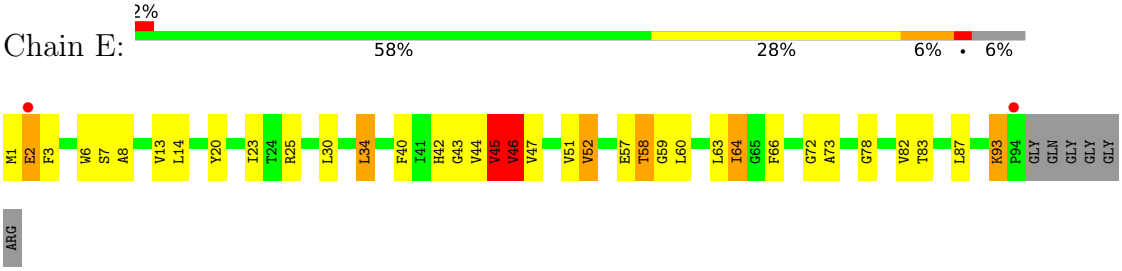
• Molecule 1: NAD(P) transhydrogenase subunit alpha 2

Chain C:



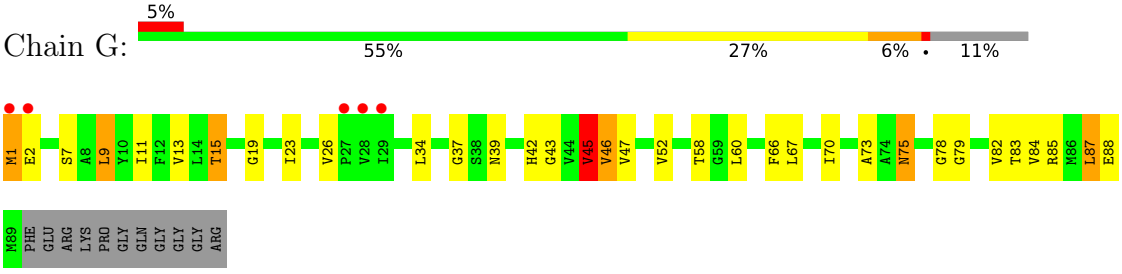
• Molecule 1: NAD(P) transhydrogenase subunit alpha 2

Chain E:



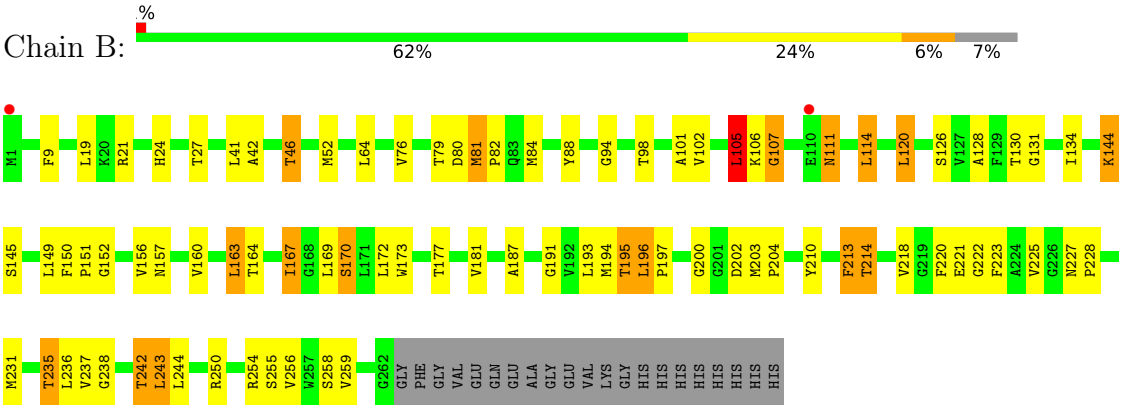
• Molecule 1: NAD(P) transhydrogenase subunit alpha 2

Chain G:



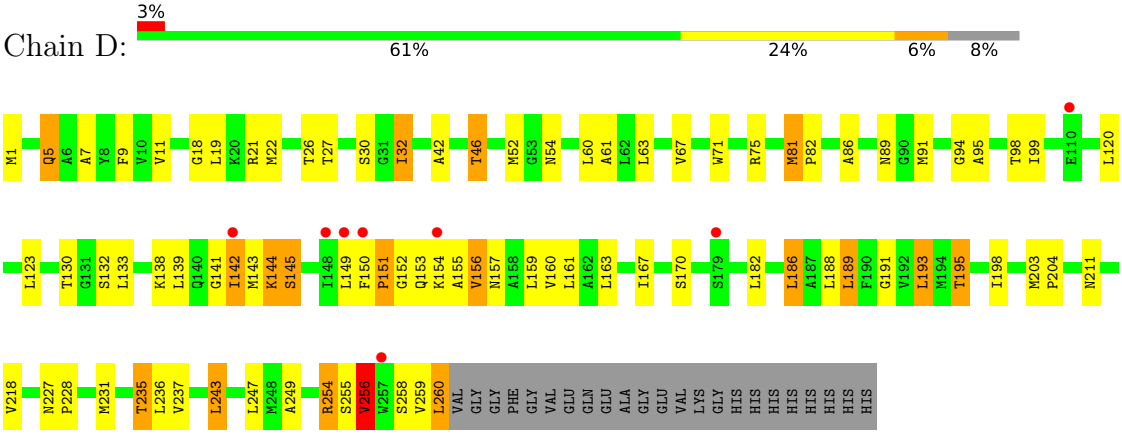
• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain B:



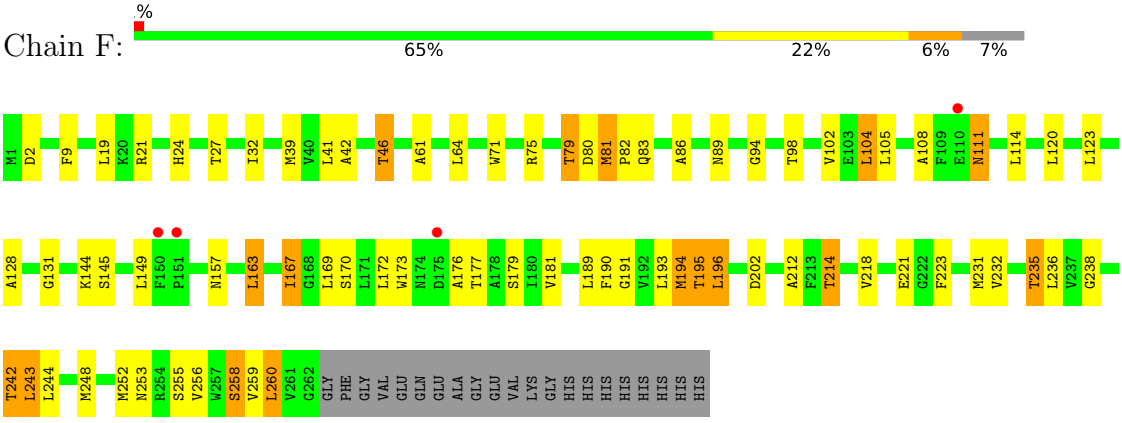
• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain D:



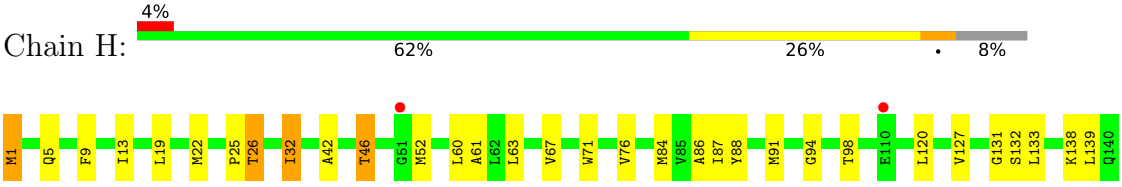
• Molecule 2: NAD(P) transhydrogenase subunit beta

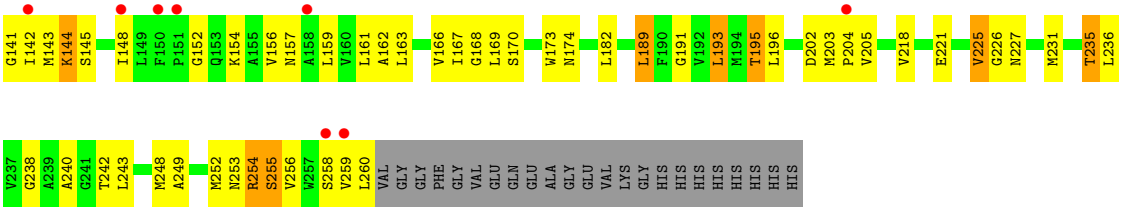
Chain F:



• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain H:




G141 I142 M143 K144 S145 I148 L149 F150 P151 G152 Q153 K154 A155 V156 N157 A158 L159 V160 L161 A162 L163 V166 I167 G168 L169 S170 W173 N174 L182 L189 F190 G191 V192 L193 M194 T195 L196 D202 M203 P204 V205 V218 E221 V225 G226 N227 M231 T235 L236
V237 G238 A239 A240 G241 T242 L243 M248 A249 M252 N253 R254 S255 V256 W257 S258 V259 L260 VAL GLY GLY PHE GLY VAL GLU GLN GLU ALA GLY GLU VAL LYS GLY HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.22Å 86.39Å 125.15Å 90.00° 93.99° 90.00°	Depositor
Resolution (Å)	46.30 – 3.08 46.30 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.30-3.08) 98.5 (46.30-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.219 , 0.280 0.233 , 0.283	Depositor DCC
R_{free} test set	1899 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	83.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.8	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	0.93	EDS
Total number of atoms	10352	wwPDB-VP
Average B, all atoms (Å^2)	74.0	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 55.04 % 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 3.3471e-05. 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

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	0.52	0/730	0.80	0/990
1	C	0.50	0/681	0.73	0/925
1	E	0.57	0/730	0.87	2/990 (0.2%)
1	G	0.54	0/681	0.79	0/925
2	B	0.57	0/1945	0.72	0/2650
2	D	0.51	0/1934	0.72	0/2635
2	F	0.55	0/1945	0.75	0/2650
2	H	0.53	0/1934	0.71	0/2635
All	All	0.54	0/10580	0.75	2/14400 (0.0%)

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
2	B	0	1
2	D	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	58	THR	N-CA-C	5.29	125.28	111.00
1	E	46	VAL	CB-CA-C	-5.22	101.47	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	105	LEU	Peptide
2	D	152	GLY	Peptide
2	H	152	GLY	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	713	0	739	23	0
1	C	666	0	691	28	0
1	E	713	0	739	21	0
1	G	666	0	691	26	0
2	B	1904	0	2018	54	0
2	D	1893	0	2006	65	0
2	F	1904	0	2018	46	0
2	H	1893	0	2006	59	0
All	All	10352	0	10908	269	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 13.

All (269) 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)
2:H:255:SER:OG	2:H:258:SER:OG	1.74	1.03
2:H:202:ASP:OD1	2:H:254:ARG:NH1	1.98	0.96
2:D:260:LEU:HD12	2:D:260:LEU:H	1.30	0.94
2:D:42:ALA:O	2:D:46:THR:HG23	1.67	0.94
2:D:254:ARG:HG3	2:D:254:ARG:HH11	1.36	0.89
2:F:231:MET:O	2:F:235:THR:HG23	1.73	0.88
1:C:87:LEU:HD23	2:D:32:ILE:HD12	1.55	0.87
2:H:255:SER:HG	2:H:258:SER:HG	1.18	0.84
2:B:163:LEU:O	2:B:167:ILE:HG22	1.77	0.84
2:H:254:ARG:HH21	2:H:258:SER:HB3	1.42	0.83
1:G:23:ILE:HD12	1:G:34:LEU:HD11	1.61	0.82
2:F:255:SER:O	2:F:258:SER:OG	1.98	0.81
1:G:11:ILE:O	1:G:15:THR:HG23	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:ARG:NH1	2:D:258:SER:OG	2.14	0.79
2:F:163:LEU:O	2:F:167:ILE:HG22	1.84	0.77
2:D:163:LEU:O	2:D:167:ILE:HD12	1.84	0.77
2:D:231:MET:O	2:D:235:THR:HG23	1.85	0.77
1:C:83:THR:HG23	2:D:32:ILE:HG21	1.67	0.76
2:D:141:GLY:HA2	2:D:144:LYS:HB3	1.68	0.76
2:H:205:VAL:HG11	2:H:259:VAL:HG21	1.70	0.73
2:D:260:LEU:HD12	2:D:260:LEU:N	2.03	0.73
1:A:57:GLU:O	1:A:59:GLY:N	2.22	0.72
2:B:231:MET:O	2:B:235:THR:HG23	1.91	0.71
1:G:87:LEU:HD23	2:H:32:ILE:HD12	1.72	0.71
2:B:24:HIS:HB2	2:B:27:THR:HG22	1.73	0.71
2:D:32:ILE:HD13	2:D:32:ILE:H	1.56	0.71
2:D:144:LYS:O	2:D:145:SER:OG	2.08	0.70
2:F:128:ALA:HB1	2:F:214:THR:HG22	1.73	0.70
2:H:252:MET:HE2	2:H:254:ARG:HG3	1.74	0.69
2:H:189:LEU:HD22	2:H:193:LEU:HD23	1.75	0.69
2:H:42:ALA:O	2:H:46:THR:HG23	1.92	0.68
2:H:94:GLY:O	2:H:98:THR:HG23	1.93	0.68
2:H:254:ARG:HH21	2:H:258:SER:CB	2.07	0.68
2:D:189:LEU:HD22	2:D:193:LEU:HD23	1.76	0.68
2:D:256:VAL:O	2:D:259:VAL:HB	1.93	0.68
2:H:191:GLY:O	2:H:195:THR:HG22	1.94	0.67
1:G:79:GLY:O	1:G:83:THR:HG22	1.94	0.67
2:B:157:ASN:OD1	2:B:193:LEU:HB3	1.94	0.66
2:F:9:PHE:CE1	1:G:9:LEU:HD13	2.31	0.66
2:D:254:ARG:HG3	2:D:254:ARG:NH1	2.07	0.66
1:C:66:PHE:CE1	1:C:70:ILE:HD11	2.30	0.66
2:D:5:GLN:HE21	2:D:5:GLN:HA	1.62	0.65
2:H:255:SER:C	2:H:256:VAL:HG23	2.17	0.65
1:E:47:VAL:HG13	2:F:46:THR:HG21	1.79	0.65
2:D:138:LYS:HA	2:D:144:LYS:HA	1.79	0.65
1:G:85:ARG:NH2	2:H:76:VAL:O	2.29	0.64
1:A:1:MET:HB2	1:A:8:ALA:HB3	1.80	0.64
2:F:24:HIS:HB2	2:F:27:THR:HG22	1.79	0.64
1:G:42:HIS:O	1:G:45:VAL:HG22	1.97	0.64
2:D:27:THR:O	2:D:30:SER:HB3	1.97	0.64
2:D:94:GLY:O	2:D:98:THR:HG23	1.97	0.64
2:F:238:GLY:O	2:F:242:THR:HG23	1.98	0.63
1:G:66:PHE:CE2	1:G:70:ILE:HD11	2.34	0.63
2:B:222:GLY:O	2:B:225:VAL:O	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:GLY:O	2:B:98:THR:HG23	1.98	0.62
2:H:249:ALA:CB	2:H:256:VAL:HG22	2.30	0.62
1:A:42:HIS:O	1:A:45:VAL:HG22	2.00	0.61
2:H:63:LEU:O	2:H:67:VAL:HG22	2.00	0.61
1:E:6:TRP:HE1	2:H:1:MET:HA	1.65	0.61
2:B:9:PHE:CE1	1:C:9:LEU:HD13	2.34	0.61
2:D:231:MET:O	2:D:235:THR:CG2	2.48	0.61
2:B:238:GLY:O	2:B:242:THR:HG23	2.01	0.61
1:E:2:GLU:HB2	2:F:223:PHE:O	2.01	0.60
2:H:131:GLY:HA2	2:H:195:THR:HG21	1.82	0.60
2:B:9:PHE:HZ	1:C:13:VAL:HG21	1.65	0.60
1:G:45:VAL:HG13	2:H:218:VAL:HG22	1.82	0.60
2:F:248:MET:O	2:F:252:MET:HG3	2.01	0.60
2:H:138:LYS:HA	2:H:144:LYS:HA	1.83	0.59
2:D:18:GLY:O	2:D:22:MET:HG3	2.03	0.59
2:B:9:PHE:CZ	1:C:9:LEU:HD13	2.38	0.59
2:B:202:ASP:HB3	2:B:259:VAL:HG13	1.84	0.58
2:H:170:SER:O	2:H:173:TRP:O	2.22	0.58
2:H:231:MET:O	2:H:235:THR:HG23	2.04	0.58
1:C:45:VAL:HG13	2:D:218:VAL:HG22	1.86	0.57
1:E:57:GLU:O	1:E:59:GLY:N	2.32	0.57
1:A:84:VAL:O	1:A:88:GLU:HG3	2.04	0.57
2:H:9:PHE:CE2	2:H:13:ILE:HD11	2.39	0.57
2:B:131:GLY:HA2	2:B:195:THR:HG21	1.87	0.56
2:D:189:LEU:CD2	2:D:193:LEU:HD23	2.35	0.56
1:E:42:HIS:O	1:E:45:VAL:HG22	2.05	0.56
1:G:46:VAL:HG13	1:G:73:ALA:N	2.20	0.56
1:E:13:VAL:HG21	2:H:9:PHE:HZ	1.71	0.56
2:F:202:ASP:HB3	2:F:259:VAL:HG13	1.88	0.56
2:H:157:ASN:OD1	2:H:193:LEU:HD12	2.06	0.56
2:H:252:MET:CE	2:H:254:ARG:HG3	2.34	0.56
2:F:42:ALA:O	2:F:46:THR:CG2	2.54	0.55
2:F:42:ALA:O	2:F:46:THR:HG22	2.06	0.55
2:D:254:ARG:HH11	2:D:254:ARG:CG	2.14	0.55
1:G:47:VAL:HG13	2:H:46:THR:HG21	1.87	0.55
1:C:87:LEU:CD2	2:D:32:ILE:HD12	2.33	0.55
2:F:89:ASN:HD21	2:F:214:THR:HG23	1.71	0.55
2:F:131:GLY:HA2	2:F:195:THR:HG21	1.89	0.55
2:H:248:MET:O	2:H:252:MET:HG3	2.07	0.55
2:D:21:ARG:HH12	2:D:27:THR:HG22	1.72	0.55
2:H:238:GLY:O	2:H:242:THR:OG1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLY:O	1:C:46:VAL:HG23	2.07	0.54
2:D:149:LEU:HA	2:D:153:GLN:OE1	2.07	0.54
2:D:95:ALA:O	2:D:99:ILE:HG13	2.07	0.54
2:B:150:PHE:HB2	2:B:151:PRO:HD2	1.90	0.54
1:A:1:MET:HB2	1:A:8:ALA:CB	2.37	0.54
2:F:79:THR:HG22	2:F:80:ASP:OD1	2.07	0.54
2:B:21:ARG:O	2:B:27:THR:HG23	2.08	0.54
2:H:205:VAL:CG1	2:H:259:VAL:HG21	2.37	0.54
2:F:94:GLY:O	2:F:98:THR:HG23	2.08	0.54
1:A:47:VAL:HG13	2:B:46:THR:HG21	1.90	0.53
2:F:193:LEU:HA	2:F:196:LEU:HD22	1.90	0.53
1:C:23:ILE:O	1:C:26:VAL:HG13	2.08	0.53
2:D:144:LYS:HG3	2:D:145:SER:N	2.22	0.53
1:E:23:ILE:HD12	1:E:34:LEU:HD11	1.89	0.53
2:B:42:ALA:O	2:B:46:THR:HG22	2.09	0.53
2:B:238:GLY:O	2:B:242:THR:CG2	2.56	0.53
2:D:156:VAL:O	2:D:160:VAL:HG23	2.09	0.53
1:A:60:LEU:O	1:A:64:ILE:HG22	2.08	0.53
1:C:47:VAL:HG13	2:D:46:THR:HG21	1.90	0.53
2:D:163:LEU:C	2:D:167:ILE:HD12	2.29	0.53
1:A:46:VAL:HG13	1:A:72:GLY:C	2.29	0.53
1:A:13:VAL:HG21	2:D:9:PHE:HZ	1.73	0.52
2:D:249:ALA:O	2:D:254:ARG:O	2.27	0.52
2:F:9:PHE:CZ	1:G:9:LEU:HD13	2.43	0.52
2:F:128:ALA:CB	2:F:214:THR:HG22	2.39	0.52
1:E:1:MET:HB2	1:E:8:ALA:HB3	1.92	0.52
2:D:81:MET:N	2:D:82:PRO:HD2	2.25	0.52
2:H:127:VAL:HG13	2:H:191:GLY:HA2	1.91	0.52
2:F:193:LEU:HA	2:F:196:LEU:CD2	2.40	0.51
2:B:193:LEU:HA	2:B:196:LEU:HD22	1.93	0.51
2:D:5:GLN:HE22	2:D:228:PRO:HG2	1.75	0.51
2:D:144:LYS:O	2:D:145:SER:CB	2.57	0.51
2:D:63:LEU:O	2:D:67:VAL:HG22	2.11	0.51
2:D:130:THR:OG1	2:D:191:GLY:HA3	2.10	0.51
1:E:47:VAL:O	1:E:51:VAL:HG23	2.10	0.51
1:E:64:ILE:CD1	2:F:102:VAL:HG23	2.40	0.51
2:B:130:THR:OG1	2:B:191:GLY:HA3	2.10	0.51
2:H:252:MET:O	2:H:253:ASN:HB2	2.09	0.51
2:H:254:ARG:NH2	2:H:258:SER:CB	2.73	0.51
2:D:157:ASN:OD1	2:D:193:LEU:HD12	2.10	0.51
1:A:64:ILE:CD1	2:B:102:VAL:HG23	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:LEU:HD22	2:D:247:LEU:HG	1.92	0.51
2:D:141:GLY:CA	2:D:144:LYS:HB3	2.40	0.50
1:E:40:PHE:CZ	2:F:39:MET:HG3	2.46	0.50
2:F:190:PHE:CE2	2:F:194:MET:HG3	2.46	0.50
2:F:191:GLY:O	2:F:195:THR:HG22	2.11	0.50
2:F:83:GLN:O	2:F:86:ALA:HB3	2.11	0.50
1:G:23:ILE:HG13	2:H:240:ALA:HB1	1.94	0.50
2:B:42:ALA:O	2:B:46:THR:CG2	2.60	0.50
1:A:2:GLU:HB2	2:B:223:PHE:O	2.11	0.50
2:H:167:ILE:O	2:H:170:SER:OG	2.23	0.50
2:B:128:ALA:HB1	2:B:214:THR:HG22	1.94	0.50
2:H:168:GLY:O	2:H:169:LEU:C	2.49	0.50
2:D:256:VAL:O	2:D:260:LEU:HD12	2.13	0.49
2:D:142:ILE:HG22	2:D:142:ILE:O	2.11	0.49
1:E:46:VAL:HG13	1:E:73:ALA:N	2.28	0.49
2:F:21:ARG:O	2:F:27:THR:HG23	2.12	0.49
1:A:50:MET:O	2:B:52:MET:HE3	2.13	0.49
1:C:47:VAL:HG22	2:D:46:THR:HG21	1.93	0.49
2:D:167:ILE:HD13	2:D:186:LEU:HD12	1.95	0.49
2:H:141:GLY:O	2:H:143:MET:N	2.46	0.49
1:E:46:VAL:HG13	1:E:72:GLY:C	2.34	0.48
2:F:238:GLY:O	2:F:242:THR:CG2	2.59	0.48
1:A:20:TYR:CE2	2:B:243:LEU:HG	2.48	0.48
2:B:210:TYR:HA	2:B:213:PHE:HB2	1.96	0.48
2:H:88:TYR:HA	2:H:91:MET:HG2	1.96	0.48
2:D:203:MET:N	2:D:204:PRO:CD	2.77	0.48
1:C:26:VAL:HG23	1:C:26:VAL:O	2.13	0.48
2:B:81:MET:N	2:B:82:PRO:CD	2.76	0.48
2:D:195:THR:HA	2:D:198:ILE:HD12	1.95	0.48
1:A:43:GLY:O	1:A:46:VAL:HG22	2.14	0.47
2:B:101:ALA:O	2:B:105:LEU:HG	2.14	0.47
1:E:1:MET:HB2	1:E:8:ALA:CB	2.43	0.47
1:G:26:VAL:HG23	1:G:26:VAL:O	2.14	0.47
1:C:11:ILE:O	1:C:15:THR:HG23	2.14	0.47
2:F:9:PHE:HZ	1:G:13:VAL:HG21	1.79	0.47
1:E:66:PHE:CE1	2:F:61:ALA:HB2	2.50	0.47
2:D:150:PHE:O	2:D:151:PRO:O	2.33	0.47
2:H:163:LEU:O	2:H:167:ILE:HD12	2.14	0.47
1:C:38:SER:HB2	2:D:237:VAL:HG13	1.97	0.47
2:F:255:SER:OG	2:F:258:SER:OG	1.76	0.47
2:B:126:SER:HB2	2:B:187:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LYS:HA	2:B:144:LYS:HE2	1.96	0.47
2:D:167:ILE:CD1	2:D:186:LEU:HD12	2.45	0.46
2:F:212:ALA:HB1	2:F:242:THR:HG22	1.98	0.46
2:H:254:ARG:NH2	2:H:258:SER:HB3	2.20	0.46
2:B:120:LEU:HD13	2:B:220:PHE:CE2	2.50	0.46
1:C:75:ASN:C	1:C:75:ASN:HD22	2.18	0.46
1:E:78:GLY:O	1:E:82:VAL:HG23	2.16	0.46
2:F:89:ASN:HD21	2:F:214:THR:CG2	2.29	0.46
1:G:42:HIS:CD2	1:G:75:ASN:OD1	2.69	0.46
2:B:214:THR:O	2:B:218:VAL:HG13	2.15	0.46
2:H:86:ALA:O	2:H:132:SER:HB3	2.16	0.46
2:H:231:MET:O	2:H:235:THR:CG2	2.63	0.46
2:D:86:ALA:O	2:D:132:SER:HB3	2.16	0.46
1:E:83:THR:HG21	2:F:32:ILE:HD13	1.98	0.46
1:A:64:ILE:HD11	2:B:98:THR:HA	1.99	0.45
2:B:167:ILE:HD13	2:B:167:ILE:C	2.36	0.45
2:H:202:ASP:CG	2:H:254:ARG:HH12	2.19	0.45
2:D:130:THR:HG23	2:D:188:LEU:HD23	1.97	0.45
1:A:47:VAL:HG22	2:B:46:THR:HG21	1.99	0.45
2:B:81:MET:HE3	2:B:84:MET:HG3	1.97	0.45
1:G:83:THR:HG23	2:H:32:ILE:HG21	1.97	0.45
1:A:82:VAL:HG13	2:B:81:MET:HG3	1.98	0.45
2:B:152:GLY:O	2:B:156:VAL:HG23	2.17	0.45
1:G:78:GLY:O	1:G:82:VAL:HG22	2.17	0.45
2:F:111:ASN:HD22	2:F:111:ASN:C	2.21	0.44
2:B:130:THR:O	2:B:134:ILE:HG12	2.18	0.44
2:D:260:LEU:H	2:D:260:LEU:CD1	2.15	0.44
2:B:167:ILE:O	2:B:170:SER:HB3	2.17	0.44
2:F:104:LEU:HD12	2:F:104:LEU:HA	1.86	0.44
1:G:70:ILE:HG13	2:H:61:ALA:HB1	1.99	0.44
2:B:203:MET:N	2:B:204:PRO:CD	2.81	0.44
2:H:193:LEU:HD13	2:H:196:LEU:HD12	1.99	0.44
1:A:52:VAL:HG13	2:B:102:VAL:HG11	2.00	0.44
2:D:21:ARG:NH1	2:D:27:THR:HG22	2.32	0.44
1:E:14:LEU:HD13	1:G:15:THR:HG22	2.00	0.43
1:G:39:ASN:HA	1:G:42:HIS:CE1	2.52	0.43
2:H:203:MET:N	2:H:204:PRO:HD2	2.33	0.43
2:D:195:THR:HA	2:D:198:ILE:CD1	2.47	0.43
2:F:255:SER:HG	2:F:258:SER:HG	0.43	0.43
1:G:84:VAL:HG22	2:H:32:ILE:HG13	2.00	0.43
2:B:111:ASN:HB3	2:B:114:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:LEU:O	1:E:34:LEU:HB2	2.18	0.43
2:F:71:TRP:O	2:F:75:ARG:HG2	2.19	0.43
1:E:20:TYR:CE2	2:F:243:LEU:HG	2.54	0.43
2:B:106:LYS:O	2:B:107:GLY:C	2.56	0.43
1:C:46:VAL:HG22	1:C:72:GLY:C	2.39	0.43
2:H:84:MET:HA	2:H:87:ILE:HG22	2.01	0.43
1:C:41:ILE:O	1:C:44:VAL:HG12	2.19	0.43
1:C:23:ILE:HD12	1:C:34:LEU:HD11	2.00	0.42
1:C:29:ILE:H	1:C:29:ILE:HD12	1.84	0.42
2:D:71:TRP:CD1	2:D:75:ARG:HD2	2.55	0.42
2:H:87:ILE:O	2:H:91:MET:HG2	2.18	0.42
2:H:193:LEU:HD13	2:H:193:LEU:HA	1.87	0.42
1:A:14:LEU:HD13	1:C:15:THR:HG22	2.02	0.42
2:H:162:ALA:O	2:H:166:VAL:HG23	2.19	0.42
2:F:176:ALA:O	2:F:179:SER:N	2.52	0.42
1:E:52:VAL:HG13	2:F:102:VAL:HG11	2.01	0.42
1:G:37:GLY:HA3	2:H:22:MET:CE	2.49	0.42
1:A:78:GLY:HA3	2:B:88:TYR:CE2	2.55	0.42
2:D:255:SER:O	2:D:258:SER:N	2.52	0.42
2:B:9:PHE:CZ	1:C:13:VAL:HG21	2.50	0.42
2:B:200:GLY:O	2:B:203:MET:HB2	2.20	0.42
2:B:160:VAL:O	2:B:164:THR:OG1	2.33	0.41
2:D:7:ALA:O	2:D:11:VAL:HG23	2.20	0.41
2:D:130:THR:HG23	2:D:188:LEU:CD2	2.50	0.41
2:F:157:ASN:OD1	2:F:193:LEU:HB3	2.20	0.41
2:H:255:SER:C	2:H:256:VAL:CG2	2.85	0.41
2:B:80:ASP:O	2:B:84:MET:HG2	2.20	0.41
1:C:42:HIS:HE1	2:D:211:ASN:OD1	2.03	0.41
1:G:1:MET:HB3	2:H:226:GLY:HA3	2.03	0.41
2:B:227:ASN:HA	2:B:228:PRO:HD3	1.86	0.41
2:F:81:MET:HA	2:F:81:MET:CE	2.50	0.41
1:C:83:THR:O	1:C:87:LEU:HD22	2.21	0.41
2:F:81:MET:N	2:F:82:PRO:CD	2.83	0.41
1:G:19:GLY:CA	2:H:236:LEU:HD22	2.50	0.41
2:D:153:GLN:C	2:D:155:ALA:N	2.72	0.41
2:H:144:LYS:O	2:H:145:SER:CB	2.68	0.41
1:C:63:LEU:O	1:C:63:LEU:HD22	2.21	0.41
2:H:141:GLY:HA2	2:H:144:LYS:HB3	2.02	0.41
2:F:260:LEU:HD12	2:F:260:LEU:HA	1.91	0.41
2:B:196:LEU:N	2:B:197:PRO:CD	2.84	0.41
2:H:221:GLU:O	2:H:225:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:HIS:HD2	2:B:237:VAL:HG11	1.86	0.40
2:D:254:ARG:NH1	2:D:254:ARG:CG	2.73	0.40
1:A:21:GLU:HG3	1:C:21:GLU:HG3	2.03	0.40
2:B:76:VAL:HG13	2:B:80:ASP:HB2	2.03	0.40
1:C:70:ILE:HG13	2:D:61:ALA:HB1	2.03	0.40
2:D:89:ASN:OD1	2:D:211:ASN:HA	2.21	0.40
1:A:64:ILE:HD13	2:B:102:VAL:HG23	2.02	0.40
2:F:214:THR:O	2:F:218:VAL:HG13	2.21	0.40
1:C:39:ASN:HA	1:C:42:HIS:CE1	2.57	0.40
1:G:23:ILE:CD1	1:G:34:LEU:HD11	2.42	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	92/100 (92%)	81 (88%)	7 (8%)	4 (4%)	2	14
1	C	87/100 (87%)	81 (93%)	4 (5%)	2 (2%)	6	26
1	E	92/100 (92%)	83 (90%)	5 (5%)	4 (4%)	2	14
1	G	87/100 (87%)	78 (90%)	6 (7%)	3 (3%)	3	19
2	B	260/283 (92%)	244 (94%)	15 (6%)	1 (0%)	34	66
2	D	258/283 (91%)	234 (91%)	18 (7%)	6 (2%)	6	26
2	F	260/283 (92%)	237 (91%)	20 (8%)	3 (1%)	13	42
2	H	258/283 (91%)	233 (90%)	20 (8%)	5 (2%)	8	31
All	All	1394/1532 (91%)	1271 (91%)	95 (7%)	28 (2%)	7	29

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR
2	D	145	SER
2	D	256	VAL
1	E	58	THR
2	H	26	THR
2	H	142	ILE
2	H	174	ASN
2	B	107	GLY
2	F	108	ALA
2	F	177	THR
1	G	2	GLU
1	G	43	GLY
2	H	148	ILE
2	D	54	ASN
2	D	143	MET
2	D	151	PRO
1	C	2	GLU
1	C	44	VAL
1	G	45	VAL
2	H	25	PRO
1	A	47	VAL
1	E	93	LYS
2	F	232	VAL
2	D	142	ILE
1	A	46	VAL
1	A	93	LYS
1	E	43	GLY
1	E	45	VAL

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	73/75 (97%)	59 (81%)	14 (19%)	1 6
1	C	68/75 (91%)	55 (81%)	13 (19%)	1 6
1	E	73/75 (97%)	59 (81%)	14 (19%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	68/75 (91%)	55 (81%)	13 (19%)	1 6
2	B	188/204 (92%)	151 (80%)	37 (20%)	1 5
2	D	187/204 (92%)	155 (83%)	32 (17%)	2 8
2	F	188/204 (92%)	150 (80%)	38 (20%)	1 5
2	H	187/204 (92%)	159 (85%)	28 (15%)	3 11
All	All	1032/1116 (92%)	843 (82%)	189 (18%)	1 7

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	7	SER
1	A	23	ILE
1	A	25	ARG
1	A	34	LEU
1	A	44	VAL
1	A	45	VAL
1	A	46	VAL
1	A	52	VAL
1	A	60	LEU
1	A	63	LEU
1	A	64	ILE
1	A	87	LEU
1	A	93	LYS
2	B	19	LEU
2	B	41	LEU
2	B	46	THR
2	B	64	LEU
2	B	79	THR
2	B	81	MET
2	B	105	LEU
2	B	111	ASN
2	B	114	LEU
2	B	120	LEU
2	B	144	LYS
2	B	145	SER
2	B	149	LEU
2	B	163	LEU
2	B	167	ILE
2	B	169	LEU

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Mol	Chain	Res	Type
2	B	170	SER
2	B	172	LEU
2	B	173	TRP
2	B	177	THR
2	B	181	VAL
2	B	194	MET
2	B	195	THR
2	B	196	LEU
2	B	213	PHE
2	B	214	THR
2	B	221	GLU
2	B	235	THR
2	B	236	LEU
2	B	242	THR
2	B	243	LEU
2	B	244	LEU
2	B	250	ARG
2	B	254	ARG
2	B	255	SER
2	B	256	VAL
2	B	258	SER
1	C	1	MET
1	C	9	LEU
1	C	15	THR
1	C	38	SER
1	C	42	HIS
1	C	45	VAL
1	C	52	VAL
1	C	57	GLU
1	C	60	LEU
1	C	67	LEU
1	C	75	ASN
1	C	87	LEU
1	C	88	GLU
2	D	1	MET
2	D	5	GLN
2	D	19	LEU
2	D	26	THR
2	D	32	ILE
2	D	46	THR
2	D	52	MET
2	D	60	LEU

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Mol	Chain	Res	Type
2	D	81	MET
2	D	91	MET
2	D	120	LEU
2	D	123	LEU
2	D	133	LEU
2	D	139	LEU
2	D	144	LYS
2	D	154	LYS
2	D	156	VAL
2	D	159	LEU
2	D	161	LEU
2	D	170	SER
2	D	182	LEU
2	D	186	LEU
2	D	189	LEU
2	D	193	LEU
2	D	195	THR
2	D	227	ASN
2	D	235	THR
2	D	236	LEU
2	D	243	LEU
2	D	254	ARG
2	D	256	VAL
2	D	260	LEU
1	E	2	GLU
1	E	3	PHE
1	E	7	SER
1	E	25	ARG
1	E	34	LEU
1	E	44	VAL
1	E	45	VAL
1	E	46	VAL
1	E	52	VAL
1	E	60	LEU
1	E	63	LEU
1	E	64	ILE
1	E	87	LEU
1	E	93	LYS
2	F	2	ASP
2	F	19	LEU
2	F	41	LEU
2	F	46	THR

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Mol	Chain	Res	Type
2	F	64	LEU
2	F	79	THR
2	F	81	MET
2	F	104	LEU
2	F	105	LEU
2	F	111	ASN
2	F	114	LEU
2	F	120	LEU
2	F	123	LEU
2	F	144	LYS
2	F	145	SER
2	F	149	LEU
2	F	163	LEU
2	F	167	ILE
2	F	169	LEU
2	F	170	SER
2	F	172	LEU
2	F	173	TRP
2	F	181	VAL
2	F	189	LEU
2	F	194	MET
2	F	195	THR
2	F	196	LEU
2	F	214	THR
2	F	221	GLU
2	F	235	THR
2	F	236	LEU
2	F	242	THR
2	F	243	LEU
2	F	244	LEU
2	F	253	ASN
2	F	256	VAL
2	F	258	SER
2	F	260	LEU
1	G	1	MET
1	G	7	SER
1	G	9	LEU
1	G	15	THR
1	G	45	VAL
1	G	46	VAL
1	G	52	VAL
1	G	58	THR

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Mol	Chain	Res	Type
1	G	60	LEU
1	G	67	LEU
1	G	75	ASN
1	G	87	LEU
1	G	88	GLU
2	H	1	MET
2	H	5	GLN
2	H	19	LEU
2	H	26	THR
2	H	32	ILE
2	H	46	THR
2	H	52	MET
2	H	60	LEU
2	H	71	TRP
2	H	120	LEU
2	H	133	LEU
2	H	139	LEU
2	H	144	LYS
2	H	154	LYS
2	H	156	VAL
2	H	159	LEU
2	H	161	LEU
2	H	182	LEU
2	H	189	LEU
2	H	193	LEU
2	H	195	THR
2	H	225	VAL
2	H	227	ASN
2	H	235	THR
2	H	243	LEU
2	H	254	ARG
2	H	255	SER
2	H	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	24	HIS
2	B	89	ASN
2	B	111	ASN
1	C	42	HIS
1	C	75	ASN

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Mol	Chain	Res	Type
2	D	5	GLN
2	D	227	ASN
2	F	24	HIS
2	F	89	ASN
2	F	111	ASN
1	G	42	HIS
2	H	5	GLN
2	H	227	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 monosaccharides 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	94/100 (94%)	-0.36	0 100 100	42, 61, 105, 132	0
1	C	89/100 (89%)	-0.05	3 (3%) 45 23	51, 74, 123, 148	0
1	E	94/100 (94%)	-0.48	2 (2%) 63 41	42, 60, 102, 141	0
1	G	89/100 (89%)	-0.11	5 (5%) 24 11	49, 71, 115, 140	0
2	B	262/283 (92%)	-0.43	2 (0%) 86 71	30, 63, 91, 127	0
2	D	260/283 (91%)	-0.22	8 (3%) 49 25	52, 80, 119, 139	0
2	F	262/283 (92%)	-0.40	4 (1%) 73 53	30, 60, 87, 119	0
2	H	260/283 (91%)	-0.18	10 (3%) 40 20	51, 79, 123, 163	0
All	All	1410/1532 (92%)	-0.29	34 (2%) 59 35	30, 69, 113, 163	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	29	ILE	4.7
2	B	1	MET	4.0
1	C	89	MET	3.7
2	H	150	PHE	3.6
1	E	2	GLU	3.1
2	D	148	ILE	2.9
1	C	29	ILE	2.9
2	H	110	GLU	2.8
1	G	28	VAL	2.7
2	H	259	VAL	2.6
2	B	110	GLU	2.6
1	G	2	GLU	2.6
2	H	151	PRO	2.6
2	F	151	PRO	2.5
2	D	257	TRP	2.5
2	D	179	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	51	GLY	2.5
2	D	142	ILE	2.4
2	H	142	ILE	2.4
2	H	204	PRO	2.4
2	F	110	GLU	2.4
2	D	154	LYS	2.3
1	C	2	GLU	2.3
1	E	94	PRO	2.3
2	D	110	GLU	2.3
2	D	149	LEU	2.3
2	F	150	PHE	2.2
1	G	1	MET	2.2
2	F	175	ASP	2.1
2	H	148	ILE	2.1
2	H	258	SER	2.1
2	D	150	PHE	2.0
2	H	158	ALA	2.0
1	G	27	PRO	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.