Full wwPDB X-ray Structure Validation Report (i)

Jun 20, 2016 – 01:51 PM EDT

PDB ID	:	5HFT
Title	:	Crystal structure of HpxW
Authors	:	Ealick, S.E.; Hicks, K.A.
Deposited on	:	2016-01-07
Resolution	:	2.65 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:

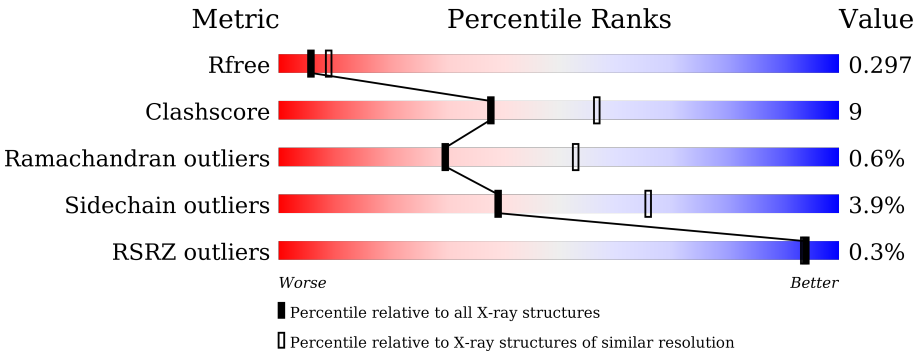
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.65 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	364	65% 19% • 16%
1	C	364	% 66% 15% • 18%
2	B	187	58% 21% • 20%
2	D	187	% 67% 16% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6380 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 Gamma-glutamyltranspeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2134	1342	383	402	7			
1	C	298	Total	C	N	O	S	0	0	0
			2064	1293	372	392	7			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A6T9C8
A	-21	GLY	-	expression tag	UNP A6T9C8
A	-20	SER	-	expression tag	UNP A6T9C8
A	-19	ASP	-	expression tag	UNP A6T9C8
A	-18	LYS	-	expression tag	UNP A6T9C8
A	-17	ILE	-	expression tag	UNP A6T9C8
A	-16	HIS	-	expression tag	UNP A6T9C8
A	-15	HIS	-	expression tag	UNP A6T9C8
A	-14	HIS	-	expression tag	UNP A6T9C8
A	-13	HIS	-	expression tag	UNP A6T9C8
A	-12	HIS	-	expression tag	UNP A6T9C8
A	-11	HIS	-	expression tag	UNP A6T9C8
A	-10	SER	-	expression tag	UNP A6T9C8
A	-9	SER	-	expression tag	UNP A6T9C8
A	-8	GLY	-	expression tag	UNP A6T9C8
A	-7	GLU	-	expression tag	UNP A6T9C8
A	-6	ASN	-	expression tag	UNP A6T9C8
A	-5	LEU	-	expression tag	UNP A6T9C8
A	-4	TYR	-	expression tag	UNP A6T9C8
A	-3	PHE	-	expression tag	UNP A6T9C8
A	-2	GLN	-	expression tag	UNP A6T9C8
A	-1	GLY	-	expression tag	UNP A6T9C8
A	0	HIS	-	expression tag	UNP A6T9C8
C	-22	MET	-	initiating methionine	UNP A6T9C8
C	-21	GLY	-	expression tag	UNP A6T9C8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	SER	-	expression tag	UNP A6T9C8
C	-19	ASP	-	expression tag	UNP A6T9C8
C	-18	LYS	-	expression tag	UNP A6T9C8
C	-17	ILE	-	expression tag	UNP A6T9C8
C	-16	HIS	-	expression tag	UNP A6T9C8
C	-15	HIS	-	expression tag	UNP A6T9C8
C	-14	HIS	-	expression tag	UNP A6T9C8
C	-13	HIS	-	expression tag	UNP A6T9C8
C	-12	HIS	-	expression tag	UNP A6T9C8
C	-11	HIS	-	expression tag	UNP A6T9C8
C	-10	SER	-	expression tag	UNP A6T9C8
C	-9	SER	-	expression tag	UNP A6T9C8
C	-8	GLY	-	expression tag	UNP A6T9C8
C	-7	GLU	-	expression tag	UNP A6T9C8
C	-6	ASN	-	expression tag	UNP A6T9C8
C	-5	LEU	-	expression tag	UNP A6T9C8
C	-4	TYR	-	expression tag	UNP A6T9C8
C	-3	PHE	-	expression tag	UNP A6T9C8
C	-2	GLN	-	expression tag	UNP A6T9C8
C	-1	GLY	-	expression tag	UNP A6T9C8
C	0	HIS	-	expression tag	UNP A6T9C8

- Molecule 2 is a protein called Gamma-glutamyltranspeptidase.

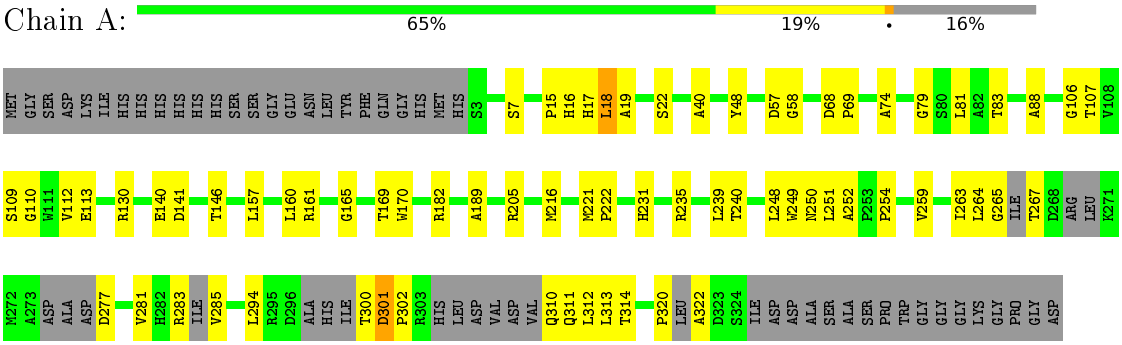
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1077	686	190	197	4			
2	D	154	Total	C	N	O	S	0	0	0
			1105	703	196	202	4			

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.

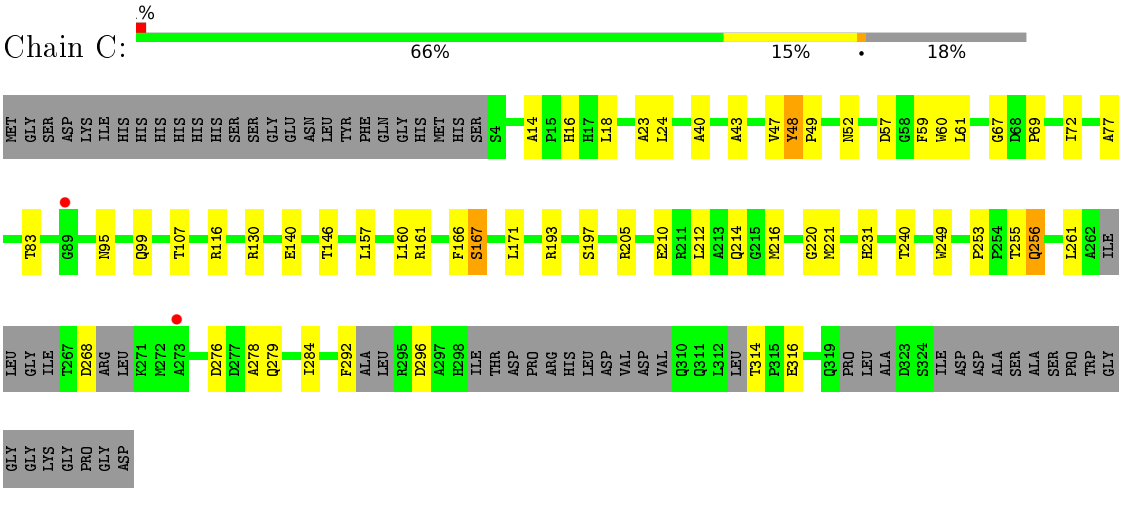
- Molecule 1: Gamma-glutamyltranspeptidase

Chain A:



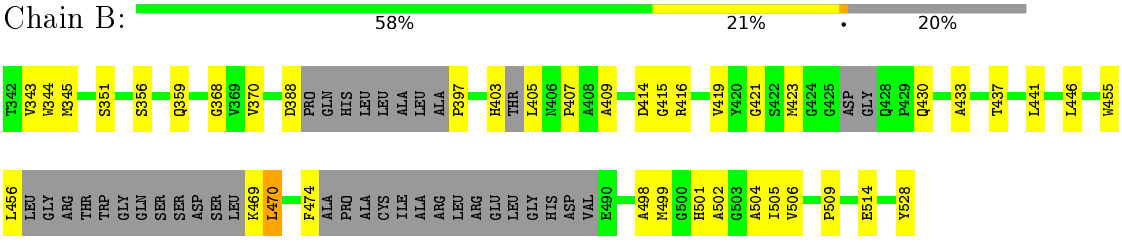
- Molecule 1: Gamma-glutamyltranspeptidase

Chain C:



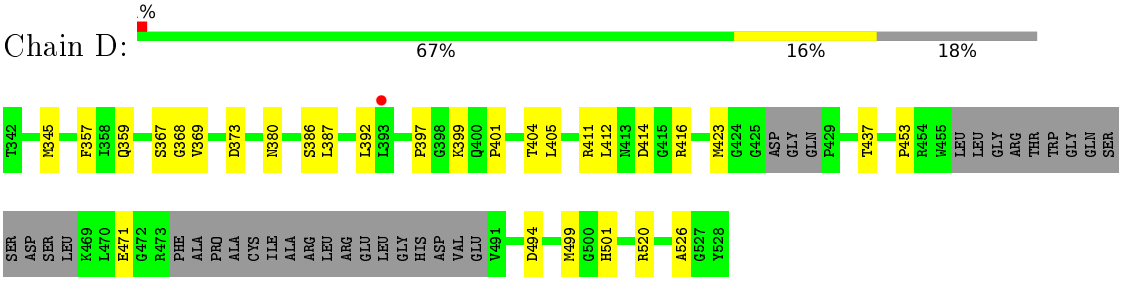
- Molecule 2: Gamma-glutamyltranspeptidase

Chain B:



• Molecule 2: Gamma-glutamyltranspeptidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.67Å 124.09Å 156.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.65 48.65 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.5 (48.65-2.65) 95.7 (48.65-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.254 , 0.298 0.254 , 0.297	Depositor DCC
R_{free} test set	1963 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6380	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 28.18 % 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 1.9294e-03. 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	0.41	0/2174	0.61	0/2971
1	C	0.40	0/2103	0.62	0/2877
2	B	0.46	0/1099	0.64	0/1486
2	D	0.41	0/1129	0.64	0/1533
All	All	0.41	0/6505	0.62	0/8867

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2134	0	2052	46	0
1	C	2064	0	1943	39	0
2	B	1077	0	1011	30	0
2	D	1105	0	1049	24	0
All	All	6380	0	6055	114	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 9.

All (114) 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:C:205:ARG:NH2	1:C:231:HIS:O	2.06	0.89
1:A:205:ARG:NH2	1:A:231:HIS:O	2.11	0.84
1:A:254:PRO:HB3	1:A:310:GLN:HG3	1.70	0.74
2:D:392:LEU:O	2:D:399:LYS:NZ	2.17	0.73
1:C:83:THR:HG22	2:D:397:PRO:HG3	1.75	0.68
2:B:403:HIS:O	2:B:405:LEU:N	2.27	0.68
1:C:99:GLN:NE2	1:C:220:GLY:O	2.25	0.68
1:A:283:ARG:O	1:A:285:VAL:N	2.29	0.66
1:A:17:HIS:CE1	1:A:18:LEU:HD13	2.31	0.66
1:C:107:THR:HG21	2:D:359:GLN:HG3	1.78	0.65
2:D:367:SER:OG	2:D:369:VAL:HG12	1.96	0.65
1:C:77:ALA:HA	2:D:401:PRO:HD3	1.77	0.65
2:B:356:SER:HB2	2:B:419:VAL:HB	1.79	0.64
1:C:253:PRO:HG2	1:C:256:GLN:HB3	1.80	0.63
1:C:130:ARG:NH1	1:C:130:ARG:O	2.31	0.63
2:B:344:TRP:CD1	2:B:421:GLY:HA3	2.34	0.63
1:A:109:SER:HA	1:A:112:VAL:HG12	1.80	0.63
1:A:312:LEU:O	1:A:314:THR:N	2.33	0.61
1:C:292:PHE:C	1:C:296:ASP:H	2.04	0.61
1:C:60:TRP:HB2	1:C:72:ILE:HB	1.83	0.61
1:A:265:GLY:O	1:A:267:THR:N	2.35	0.59
1:A:294:LEU:HD21	1:A:312:LEU:HD11	1.85	0.58
2:B:423:MET:HG2	2:B:501:HIS:HB2	1.86	0.58
1:A:130:ARG:NH1	1:A:130:ARG:O	2.37	0.57
1:C:276:ASP:HB3	1:C:279:GLN:H	1.70	0.56
1:C:16:HIS:CE1	1:C:47:VAL:HG11	2.40	0.56
1:C:216:MET:HG2	1:C:221:MET:HE3	1.88	0.55
1:A:74:ALA:O	1:A:106:GLY:HA3	2.07	0.55
1:A:141:ASP:O	1:A:182:ARG:NE	2.33	0.55
1:A:320:PRO:O	1:A:322:ALA:N	2.39	0.55
1:A:16:HIS:HE1	1:A:18:LEU:HD22	1.71	0.55
1:A:251:LEU:HB3	2:B:407:PRO:HD2	1.88	0.55
2:D:357:PHE:CZ	2:D:359:GLN:HB2	2.42	0.55
1:A:83:THR:HA	2:B:397:PRO:HG3	1.90	0.54
1:A:157:LEU:O	1:A:161:ARG:HB2	2.08	0.54
1:A:57:ASP:C	1:A:107:THR:HG23	2.30	0.52
1:C:83:THR:HG22	2:D:397:PRO:CG	2.40	0.52
1:A:259:VAL:O	1:A:263:ILE:HG13	2.09	0.52
1:A:69:PRO:HG3	1:A:249:TRP:CE2	2.45	0.52
1:A:310:GLN:O	1:A:312:LEU:N	2.41	0.52
1:C:253:PRO:HD3	2:D:404:THR:HG22	1.90	0.52
2:B:469:LYS:O	2:B:470:LEU:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:OE2	1:A:235:ARG:NH1	2.32	0.51
2:D:367:SER:HB3	2:D:380:ASN:HB3	1.93	0.51
1:C:140:GLU:HG2	1:C:193:ARG:HH22	1.75	0.51
1:A:15:PRO:HG2	2:B:343:VAL:HG22	1.93	0.51
2:B:433:ALA:O	2:B:437:THR:HG22	2.11	0.51
1:C:284:ILE:HD11	2:D:437:THR:HG21	1.93	0.50
1:C:216:MET:HA	1:C:221:MET:HE2	1.94	0.50
1:A:107:THR:HG21	2:B:359:GLN:HG3	1.93	0.49
1:C:47:VAL:C	1:C:49:PRO:HD3	2.33	0.49
1:A:165:GLY:HA3	2:B:370:VAL:HB	1.95	0.49
1:A:216:MET:HG2	1:A:221:MET:HE1	1.94	0.49
1:A:216:MET:HA	1:A:221:MET:HE3	1.95	0.49
2:B:430:GLN:OE1	2:B:455:TRP:NE1	2.39	0.49
1:C:57:ASP:C	1:C:107:THR:HG23	2.33	0.48
1:A:301:ASP:HB2	1:A:302:PRO:HD2	1.96	0.48
1:A:19:ALA:HB1	2:B:345:MET:HE1	1.95	0.48
1:A:249:TRP:C	1:A:250:ASN:HD22	2.18	0.47
1:C:23:ALA:HB2	1:C:40:ALA:HB2	1.97	0.47
1:A:248:LEU:HD12	2:B:409:ALA:O	2.16	0.46
1:A:40:ALA:HB1	2:B:345:MET:HE1	1.96	0.46
1:C:253:PRO:HD3	2:D:404:THR:CG2	2.45	0.46
1:C:67:GLY:O	2:D:411:ARG:NH1	2.35	0.46
2:B:421:GLY:O	2:B:502:ALA:HA	2.15	0.46
2:D:453:PRO:HA	2:D:520:ARG:NH2	2.30	0.46
1:A:48:TYR:HE1	1:A:146:THR:HG21	1.82	0.45
1:C:61:LEU:HD21	1:C:249:TRP:HB2	1.98	0.45
1:C:69:PRO:HG3	1:C:249:TRP:CE2	2.50	0.45
2:D:386:SER:O	2:D:387:LEU:HD23	2.17	0.45
2:B:505:ILE:HA	2:B:514:GLU:O	2.17	0.45
1:C:212:LEU:O	1:C:216:MET:HG3	2.16	0.44
1:A:79:GLY:HA3	1:A:222:PRO:O	2.17	0.44
1:C:261:LEU:HA	1:C:261:LEU:HD23	1.79	0.44
1:C:59:PHE:CD2	2:D:405:LEU:HB2	2.53	0.44
1:A:48:TYR:CE1	1:A:146:THR:HG21	2.53	0.44
2:D:471:GLU:CD	2:D:499:MET:HG3	2.37	0.44
1:A:239:LEU:HD13	1:A:252:ALA:O	2.18	0.44
1:A:281:VAL:HG23	2:B:455:TRP:CD2	2.53	0.44
1:C:16:HIS:HE1	1:C:18:LEU:HD12	1.83	0.43
2:B:437:THR:O	2:B:441:LEU:HB2	2.18	0.43
2:D:411:ARG:O	2:D:412:LEU:HD23	2.19	0.43
1:C:276:ASP:C	1:C:278:ALA:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LEU:HD13	2:D:526:ALA:O	2.19	0.43
2:D:423:MET:HG2	2:D:501:HIS:O	2.19	0.43
1:C:167:SER:O	1:C:171:LEU:HB2	2.19	0.42
1:A:264:LEU:HD21	2:B:433:ALA:HA	2.00	0.42
2:B:423:MET:CG	2:B:501:HIS:HB2	2.47	0.42
1:C:210:GLU:O	1:C:214:GLN:HG3	2.19	0.42
1:C:160:LEU:HD13	1:C:166:PHE:CE1	2.55	0.42
1:C:157:LEU:O	1:C:161:ARG:HB2	2.20	0.42
1:A:169:THR:HG22	1:A:170:TRP:CE2	2.55	0.41
1:A:58:GLY:HA3	1:A:107:THR:HG22	2.02	0.41
2:B:446:LEU:HD22	2:B:506:VAL:HG23	2.02	0.41
1:A:7:SER:HB2	2:B:528:TYR:O	2.20	0.41
2:D:373:ASP:N	2:D:373:ASP:OD1	2.53	0.41
2:B:470:LEU:HD23	2:B:474:PHE:CD2	2.56	0.41
1:A:69:PRO:HG3	1:A:249:TRP:CD2	2.55	0.41
1:A:160:LEU:HD22	2:B:368:GLY:HA3	2.01	0.41
2:B:456:LEU:HD11	2:B:498:ALA:O	2.21	0.41
2:B:419:VAL:O	2:B:504:ALA:HA	2.21	0.41
2:D:453:PRO:HB2	2:D:471:GLU:HB2	2.01	0.41
2:B:414:ASP:OD1	2:B:416:ARG:HG3	2.21	0.41
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.90	0.41
1:A:107:THR:O	1:A:110:GLY:N	2.54	0.41
1:A:301:ASP:HB2	1:A:302:PRO:CD	2.50	0.40
2:D:414:ASP:OD2	2:D:416:ARG:NH2	2.54	0.40
2:B:415:GLY:HA3	2:B:509:PRO:HG3	2.03	0.40
1:C:48:TYR:CE1	1:C:146:THR:HG21	2.56	0.40
1:C:43:ALA:O	1:C:47:VAL:HG23	2.21	0.40
1:A:140:GLU:HG2	1:A:189:ALA:CB	2.52	0.40
1:A:264:LEU:CD2	2:B:433:ALA:HA	2.52	0.40
1:C:14:ALA:HA	2:D:345:MET:HG2	2.04	0.40
1:C:160:LEU:HD22	2:D:368:GLY:HA3	2.03	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	289/364 (79%)	278 (96%)	7 (2%)	4 (1%)	14 26
1	C	284/364 (78%)	265 (93%)	18 (6%)	1 (0%)	39 63
2	B	137/187 (73%)	131 (96%)	6 (4%)	0	100 100
2	D	146/187 (78%)	140 (96%)	6 (4%)	0	100 100
All	All	856/1102 (78%)	814 (95%)	37 (4%)	5 (1%)	30 53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ALA
1	A	301	ASP
1	A	313	LEU
1	A	311	GLN
1	C	316	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	199/269 (74%)	192 (96%)	7 (4%)	43 69
1	C	186/269 (69%)	175 (94%)	11 (6%)	24 45
2	B	102/143 (71%)	98 (96%)	4 (4%)	39 66
2	D	105/143 (73%)	104 (99%)	1 (1%)	82 93
All	All	592/824 (72%)	569 (96%)	23 (4%)	39 66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	22	SER
1	A	68	ASP

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Mol	Chain	Res	Type
1	A	81	LEU
1	A	240	THR
1	A	277	ASP
1	A	300	THR
1	C	48	TYR
1	C	52	ASN
1	C	95	ASN
1	C	116	ARG
1	C	167	SER
1	C	197	SER
1	C	240	THR
1	C	255	THR
1	C	256	GLN
1	C	268	ASP
1	C	314	THR
2	B	351	SER
2	B	388	ASP
2	B	470	LEU
2	B	499	MET
2	D	494	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
2	B	432	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 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	305/364 (83%)	0.01	0 100 100	26, 42, 64, 71	0
1	C	298/364 (81%)	-0.08	2 (0%) 89 87	28, 40, 71, 85	0
2	B	149/187 (79%)	-0.13	0 100 100	30, 42, 58, 71	0
2	D	154/187 (82%)	-0.17	1 (0%) 90 89	31, 43, 65, 73	0
All	All	906/1102 (82%)	-0.07	3 (0%) 94 94	26, 41, 66, 85	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	393	LEU	2.8
1	C	89	GLY	2.5
1	C	273	ALA	2.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.