Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 07:58 AM GMT

PDB ID	:	3CVF
Title	:	Crystal Structure of the carboxy terminus of Homer3
Authors	:	Hayashi, M.K.; Stearns, M.H.; Giannini, V.; Xu, R.-M.; Sala, C.; Hayashi, Y.
Deposited on	:	2008-04-18
Resolution	:	2.90 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:

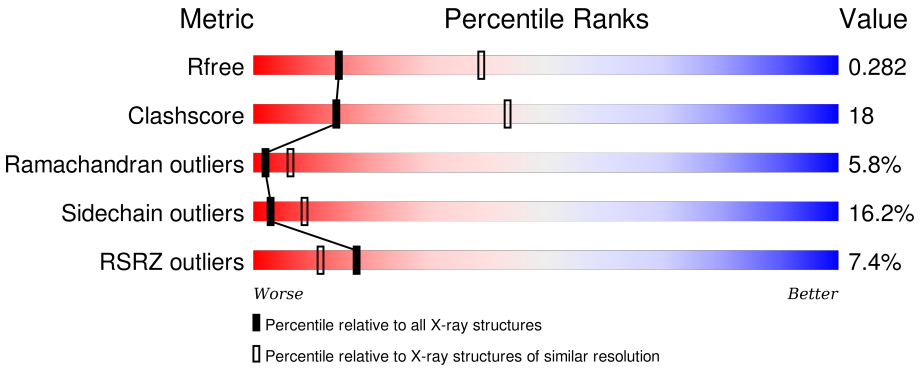
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	79	% 56% 29% • • 11%
1	B	79	4% 52% 32% • • 11%
1	C	79	13% 56% 24% 11% • 6%
1	D	79	9% 56% 24% 9% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2306 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 Homer protein homolog 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	70	Total	C	N	O	Se	0	0	0
			559	336	109	113	1			
1	B	70	Total	C	N	O	Se	0	0	0
			559	336	109	113	1			
1	C	74	Total	C	N	O	Se	0	0	0
			591	353	116	121	1			
1	D	72	Total	C	N	O	Se	0	0	0
			579	347	114	117	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLY	-	EXPRSSION TAG	UNP Q9NSC5
A	284	SER	-	EXPRSSION TAG	UNP Q9NSC5
A	285	HIS	-	EXPRSSION TAG	UNP Q9NSC5
A	286	MSE	-	EXPRSSION TAG	UNP Q9NSC5
B	283	GLY	-	EXPRSSION TAG	UNP Q9NSC5
B	284	SER	-	EXPRSSION TAG	UNP Q9NSC5
B	285	HIS	-	EXPRSSION TAG	UNP Q9NSC5
B	286	MSE	-	EXPRSSION TAG	UNP Q9NSC5
C	283	GLY	-	EXPRSSION TAG	UNP Q9NSC5
C	284	SER	-	EXPRSSION TAG	UNP Q9NSC5
C	285	HIS	-	EXPRSSION TAG	UNP Q9NSC5
C	286	MSE	-	EXPRSSION TAG	UNP Q9NSC5
D	283	GLY	-	EXPRSSION TAG	UNP Q9NSC5
D	284	SER	-	EXPRSSION TAG	UNP Q9NSC5
D	285	HIS	-	EXPRSSION TAG	UNP Q9NSC5
D	286	MSE	-	EXPRSSION TAG	UNP Q9NSC5

- Molecule 2 is water.

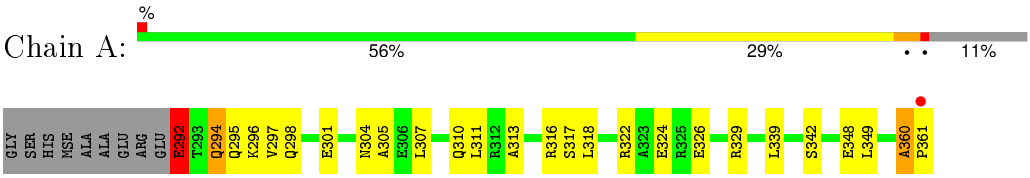
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	6	Total O 6 6	0	0
2	C	4	Total O 4 4	0	0
2	D	3	Total O 3 3	0	0

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.

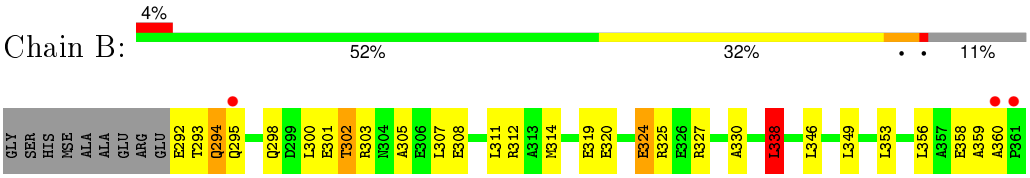
- Molecule 1: Homer protein homolog 3

Chain A:



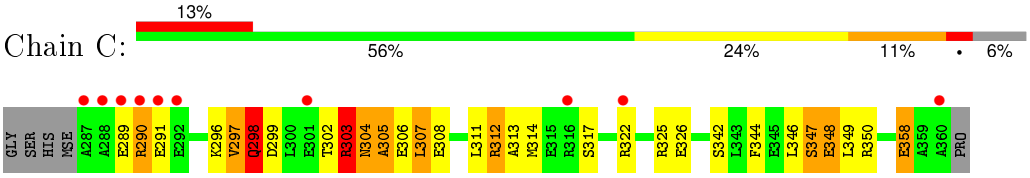
- Molecule 1: Homer protein homolog 3

Chain B:



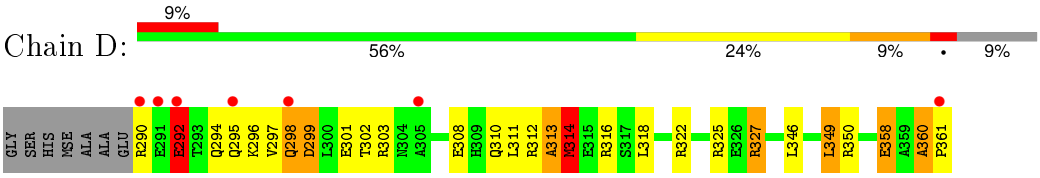
- Molecule 1: Homer protein homolog 3

Chain C:



- Molecule 1: Homer protein homolog 3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	172.03Å 172.03Å 66.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.73 – 2.90 19.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.73-2.90) 99.5 (19.73-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.75 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.252 , 0.287 0.249 , 0.282	Depositor DCC
R_{free} test set	1269 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.3	EDS
Estimated twinning fraction	0.041 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 24972 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2306	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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	1.43	4/560 (0.7%)	1.08	3/748 (0.4%)
1	B	1.24	2/560 (0.4%)	1.20	3/748 (0.4%)
1	C	1.25	6/591 (1.0%)	1.20	3/788 (0.4%)
1	D	1.16	1/580 (0.2%)	1.11	2/774 (0.3%)
All	All	1.27	13/2291 (0.6%)	1.15	11/3058 (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	A	0	1
1	C	0	1
All	All	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	ALA	C-O	-15.22	0.94	1.23
1	A	348	GLU	CG-CD	8.31	1.64	1.51
1	A	342	SER	CB-OG	7.97	1.52	1.42
1	B	319	GLU	CG-CD	7.89	1.63	1.51
1	D	358	GLU	CG-CD	7.59	1.63	1.51
1	C	344	PHE	CE1-CZ	7.29	1.51	1.37
1	C	348	GLU	CG-CD	6.77	1.62	1.51
1	C	344	PHE	CE2-CZ	6.41	1.49	1.37
1	C	344	PHE	CG-CD2	6.06	1.47	1.38
1	A	329	ARG	CG-CD	5.38	1.65	1.51
1	C	347	SER	CB-OG	-5.30	1.35	1.42
1	C	358	GLU	CG-CD	5.26	1.59	1.51
1	B	330	ALA	CA-CB	-5.12	1.41	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	350	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	B	311	LEU	CA-CB-CG	7.00	131.39	115.30
1	C	350	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	303	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	342	SER	CB-CA-C	5.71	120.94	110.10
1	B	325	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	360	ALA	C-N-CD	-5.59	108.29	120.60
1	B	338	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	C	350	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	A	294	GLN	N-CA-C	-5.05	97.37	111.00
1	D	349	LEU	CB-CG-CD1	-5.03	102.44	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	GLU	Peptide
1	C	290	ARG	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	559	0	555	13	0
1	B	559	0	555	21	2
1	C	591	0	583	28	1
1	D	579	0	574	32	1
2	A	5	0	0	0	0
2	B	6	0	0	1	0
2	C	4	0	0	0	0
2	D	3	0	0	3	0
All	All	2306	0	2267	83	2

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 18.

All (83) 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:307:LEU:HD21	1:D:308:GLU:OE2	1.40	1.18
1:C:314:MSE:HB3	1:D:314:MSE:HE2	1.43	0.96
1:C:303:ARG:O	1:C:303:ARG:HG3	1.69	0.91
1:C:311:LEU:HD23	1:D:311:LEU:HD12	1.54	0.89
1:C:314:MSE:HB3	1:D:314:MSE:CE	2.03	0.88
1:A:307:LEU:HD21	1:B:308:GLU:OE2	1.73	0.88
1:B:338:LEU:HD23	1:B:338:LEU:C	1.94	0.88
1:B:294:GLN:O	1:B:298:GLN:HG2	1.74	0.86
1:D:327:ARG:HG2	1:D:327:ARG:HH11	1.39	0.85
1:B:312:ARG:HG2	2:B:15:HOH:O	1.77	0.83
1:A:301:GLU:OE1	1:B:300:LEU:HD11	1.79	0.82
1:C:304:ASN:O	1:C:306:GLU:N	2.14	0.80
1:C:349:LEU:O	1:C:349:LEU:HD12	1.86	0.76
1:C:308:GLU:HB3	1:C:312:ARG:NH1	2.00	0.76
1:B:338:LEU:CD2	1:B:338:LEU:C	2.55	0.75
1:C:303:ARG:O	1:C:303:ARG:CG	2.35	0.73
1:C:308:GLU:HB3	1:C:312:ARG:HH12	1.54	0.71
1:D:295:GLN:HG3	1:D:296:LYS:N	2.05	0.71
1:B:338:LEU:HD23	1:B:338:LEU:O	1.90	0.70
1:D:295:GLN:HG3	1:D:296:LYS:H	1.57	0.69
1:A:298:GLN:HA	1:A:298:GLN:OE1	1.93	0.69
1:B:356:LEU:HD23	1:B:356:LEU:H	1.59	0.67
1:A:292:GLU:HA	1:A:295:GLN:HB2	1.76	0.66
1:D:297:VAL:HG12	1:D:301:GLU:OE1	1.96	0.65
1:B:292:GLU:HG3	1:B:293:THR:H	1.62	0.64
1:D:349:LEU:HD12	1:D:349:LEU:C	2.18	0.64
1:D:349:LEU:HD12	1:D:349:LEU:O	1.96	0.64
1:B:356:LEU:N	1:B:356:LEU:HD23	2.14	0.63
1:A:318:LEU:HD13	1:A:322:ARG:NH2	2.14	0.63
1:C:311:LEU:O	1:C:313:ALA:N	2.31	0.63
1:A:310:GLN:O	1:A:313:ALA:HB3	1.99	0.62
1:B:293:THR:O	1:B:295:GLN:N	2.34	0.60
1:D:313:ALA:O	1:D:316:ARG:N	2.35	0.59
1:B:293:THR:C	1:B:295:GLN:H	2.05	0.59
1:C:349:LEU:C	1:C:349:LEU:HD12	2.21	0.58
1:C:303:ARG:HH11	1:C:303:ARG:HG3	1.67	0.58
1:C:297:VAL:HG12	1:C:298:GLN:N	2.19	0.58
1:B:358:GLU:O	1:B:360:ALA:N	2.36	0.58
1:C:314:MSE:HA	1:C:314:MSE:HE2	1.86	0.57
1:C:311:LEU:C	1:C:313:ALA:H	2.07	0.57
1:C:307:LEU:CD2	1:D:308:GLU:OE2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:MSE:C	1:D:314:MSE:HE1	2.25	0.56
1:D:327:ARG:HG2	1:D:327:ARG:NH1	2.17	0.55
1:D:298:GLN:HA	1:D:301:GLU:CD	2.26	0.55
1:D:303:ARG:CB	2:D:17:HOH:O	2.55	0.54
1:C:304:ASN:O	1:C:305:ALA:C	2.46	0.54
1:C:346:LEU:O	1:C:349:LEU:HB3	2.08	0.53
1:A:307:LEU:HD11	1:B:308:GLU:OE2	2.08	0.53
1:B:293:THR:C	1:B:295:GLN:N	2.61	0.53
1:D:294:GLN:O	1:D:294:GLN:HG3	2.09	0.53
1:C:311:LEU:CD2	1:D:311:LEU:HD12	2.33	0.53
1:D:290:ARG:N	1:D:292:GLU:HB3	2.22	0.53
1:A:295:GLN:OE1	1:A:295:GLN:HA	2.09	0.51
1:D:303:ARG:HB2	2:D:17:HOH:O	2.12	0.50
1:D:313:ALA:O	1:D:314:MSE:C	2.51	0.49
1:C:311:LEU:C	1:C:313:ALA:N	2.66	0.49
1:A:295:GLN:O	1:A:296:LYS:C	2.51	0.49
1:B:292:GLU:HG3	1:B:293:THR:N	2.25	0.48
1:C:303:ARG:HG3	1:C:303:ARG:NH1	2.28	0.48
1:B:356:LEU:CD2	1:B:356:LEU:H	2.26	0.48
1:D:346:LEU:O	1:D:349:LEU:HB3	2.15	0.46
1:B:346:LEU:HA	1:B:346:LEU:HD23	1.80	0.46
1:D:296:LYS:HA	1:D:299:ASP:HB3	1.97	0.46
1:C:297:VAL:O	1:C:299:ASP:N	2.49	0.46
1:C:297:VAL:HG23	1:D:297:VAL:HG23	1.97	0.45
1:A:349:LEU:C	1:A:349:LEU:HD23	2.35	0.45
1:A:360:ALA:HB1	1:A:361:PRO:C	2.37	0.45
1:D:318:LEU:HD21	1:D:322:ARG:HH22	1.82	0.45
1:D:310:GLN:O	1:D:313:ALA:HB3	2.17	0.44
1:D:327:ARG:HH11	1:D:327:ARG:CG	2.18	0.44
1:B:324:GLU:HG2	1:B:327:ARG:HH21	1.82	0.44
1:D:318:LEU:HD21	1:D:322:ARG:NH2	2.33	0.44
1:C:302:THR:O	1:C:306:GLU:HB2	2.18	0.43
1:C:304:ASN:C	1:C:306:GLU:N	2.72	0.43
1:A:339:LEU:HA	1:A:339:LEU:HD23	1.90	0.43
1:D:303:ARG:HB3	2:D:17:HOH:O	2.17	0.42
1:A:298:GLN:CA	1:A:298:GLN:OE1	2.66	0.41
1:D:290:ARG:CB	1:D:290:ARG:CZ	2.98	0.41
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.83	0.41
1:D:360:ALA:O	1:D:361:PRO:O	2.38	0.41
1:C:297:VAL:CG1	1:C:298:GLN:N	2.84	0.41
1:B:298:GLN:HA	1:B:301:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:GLN:HA	1:D:301:GLU:OE1	2.21	0.40

All (2) 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:B:302:THR:CG2	1:D:301:GLU:OE2[6_554]	2.11	0.09
1:B:308:GLU:OE1	1:C:303:ARG:CD[6_554]	2.12	0.08

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	68/79 (86%)	61 (90%)	6 (9%)	1 (2%)	13	42
1	B	68/79 (86%)	57 (84%)	7 (10%)	4 (6%)	2	6
1	C	72/79 (91%)	50 (69%)	15 (21%)	7 (10%)	1	2
1	D	70/79 (89%)	61 (87%)	5 (7%)	4 (6%)	2	6
All	All	278/316 (88%)	229 (82%)	33 (12%)	16 (6%)	2	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	GLN
1	B	359	ALA
1	C	305	ALA
1	C	307	LEU
1	C	312	ARG
1	D	292	GLU
1	B	307	LEU
1	C	298	GLN

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Mol	Chain	Res	Type
1	A	304	ASN
1	B	305	ALA
1	C	291	GLU
1	C	296	LYS
1	D	314	MSE
1	C	304	ASN
1	D	313	ALA
1	D	360	ALA

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	56/60 (93%)	48 (86%)	8 (14%)	4 12
1	B	56/60 (93%)	49 (88%)	7 (12%)	6 17
1	C	58/60 (97%)	45 (78%)	13 (22%)	1 3
1	D	58/60 (97%)	49 (84%)	9 (16%)	3 10
All	All	228/240 (95%)	191 (84%)	37 (16%)	3 9

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	GLU
1	A	294	GLN
1	A	297	VAL
1	A	311	LEU
1	A	316	ARG
1	A	317	SER
1	A	324	GLU
1	A	326	GLU
1	B	302	THR
1	B	303	ARG
1	B	314	MSE
1	B	320	GLU
1	B	324	GLU

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Mol	Chain	Res	Type
1	B	338	LEU
1	B	349	LEU
1	C	289	GLU
1	C	290	ARG
1	C	297	VAL
1	C	298	GLN
1	C	303	ARG
1	C	317	SER
1	C	322	ARG
1	C	325	ARG
1	C	326	GLU
1	C	342	SER
1	C	347	SER
1	C	348	GLU
1	C	358	GLU
1	D	292	GLU
1	D	298	GLN
1	D	299	ASP
1	D	302	THR
1	D	312	ARG
1	D	314	MSE
1	D	325	ARG
1	D	327	ARG
1	D	358	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	69/79 (87%)	0.20	1 (1%) 78 76	25, 47, 83, 89	0
1	B	69/79 (87%)	0.33	3 (4%) 39 32	24, 48, 93, 94	0
1	C	73/79 (92%)	0.39	10 (13%) 4 2	25, 62, 96, 101	0
1	D	71/79 (89%)	0.40	7 (9%) 9 5	26, 58, 94, 98	0
All	All	282/316 (89%)	0.33	21 (7%) 17 11	24, 54, 93, 101	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	PRO	5.6
1	C	288	ALA	4.8
1	A	361	PRO	3.9
1	C	287	ALA	3.7
1	D	290	ARG	3.6
1	C	289	GLU	3.5
1	D	361	PRO	3.4
1	D	295	GLN	3.0
1	C	292	GLU	2.8
1	D	298	GLN	2.7
1	B	295	GLN	2.6
1	C	291	GLU	2.6
1	C	290	ARG	2.5
1	B	360	ALA	2.4
1	D	291	GLU	2.3
1	C	360	ALA	2.3
1	C	322	ARG	2.2
1	D	305	ALA	2.2
1	D	292	GLU	2.2
1	C	316	ARG	2.1
1	C	301	GLU	2.1

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.