



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:40 AM GMT

PDB ID : 3O4X  
Title : Crystal structure of complex between amino and carboxy terminal fragments of mDia1  
Authors : Eck, M.J.; Nezami, A.; Toms, A.V.  
Deposited on : 2010-07-27  
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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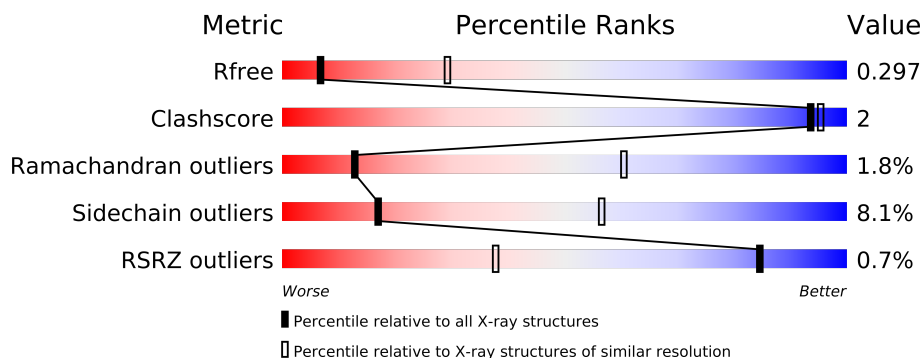
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	330	
1	B	330	
1	C	330	
1	D	330	
2	E	467	
2	F	467	
2	G	467	
2	H	467	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24335 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2552	1605	440	485	22			
1	B	318	Total	C	N	O	S	0	0	0
			2559	1609	441	487	22			
1	C	311	Total	C	N	O	S	0	0	0
			2508	1579	432	475	22			
1	D	319	Total	C	N	O	S	0	0	0
			2568	1614	442	490	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLY	-	EXPRESSION TAG	UNP O08808
A	130	SER	-	EXPRESSION TAG	UNP O08808
B	129	GLY	-	EXPRESSION TAG	UNP O08808
B	130	SER	-	EXPRESSION TAG	UNP O08808
C	129	GLY	-	EXPRESSION TAG	UNP O08808
C	130	SER	-	EXPRESSION TAG	UNP O08808
D	129	GLY	-	EXPRESSION TAG	UNP O08808
D	130	SER	-	EXPRESSION TAG	UNP O08808

- Molecule 2 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			
2	H	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			
2	G	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			
2	F	433	Total	C	N	O	S	0	0	0
			3525	2230	602	672	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	734	GLY	-	EXPRESSION TAG	UNP O08808
E	735	SER	-	EXPRESSION TAG	UNP O08808
H	734	GLY	-	EXPRESSION TAG	UNP O08808
H	735	SER	-	EXPRESSION TAG	UNP O08808
G	734	GLY	-	EXPRESSION TAG	UNP O08808
G	735	SER	-	EXPRESSION TAG	UNP O08808
F	734	GLY	-	EXPRESSION TAG	UNP O08808
F	735	SER	-	EXPRESSION TAG	UNP O08808

- Molecule 3 is water.

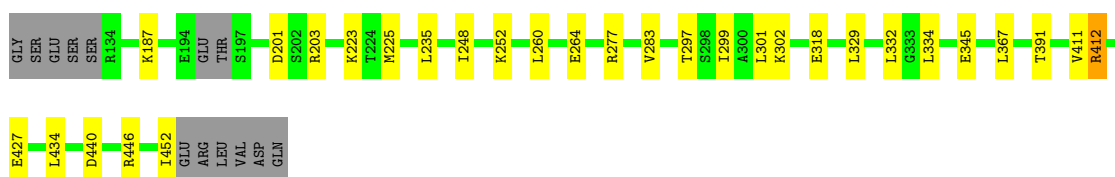
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	9	Total O 9 9	0	0
3	C	6	Total O 6 6	0	0
3	D	8	Total O 8 8	0	0
3	E	5	Total O 5 5	0	0
3	H	4	Total O 4 4	0	0
3	G	6	Total O 6 6	0	0
3	F	2	Total O 2 2	0	0

### 3 Residue-property plots

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.

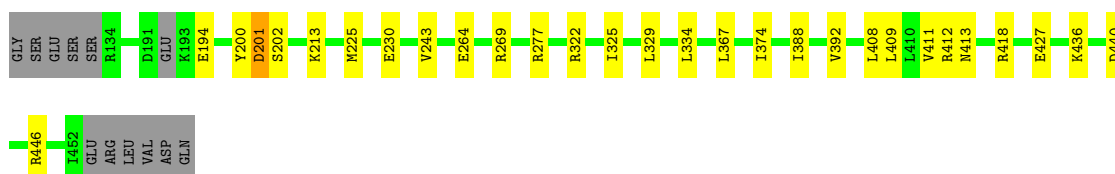
- Molecule 1: Protein diaphanous homolog 1

Chain A: 



- Molecule 1: Protein diaphanous homolog 1

Chain B: 



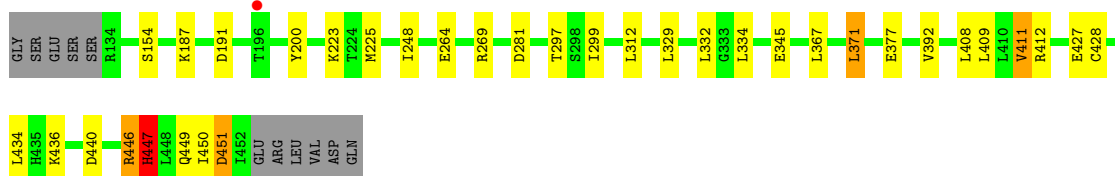
- Molecule 1: Protein diaphanous homolog 1

Chain C: 



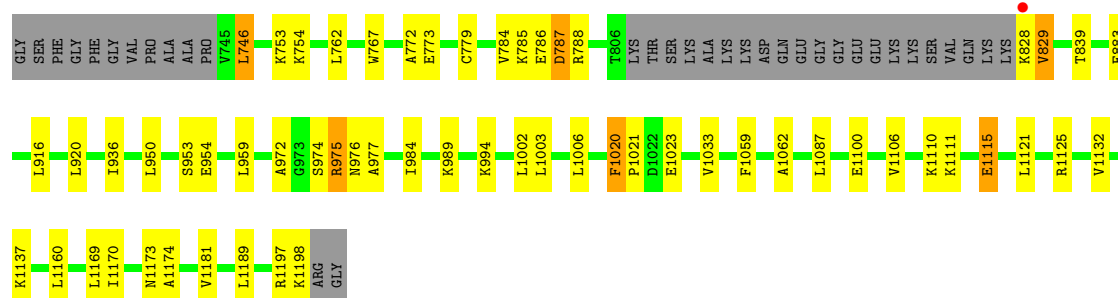
- Molecule 1: Protein diaphanous homolog 1

Chain D: 



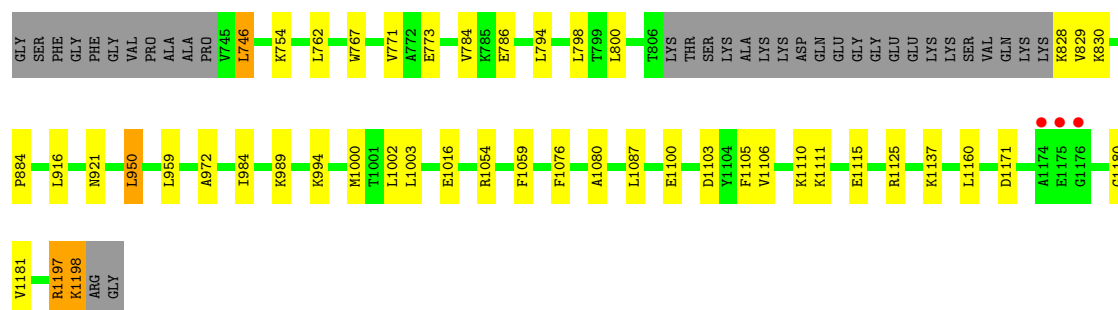
- Molecule 2: Protein diaphanous homolog 1

## Chain E:



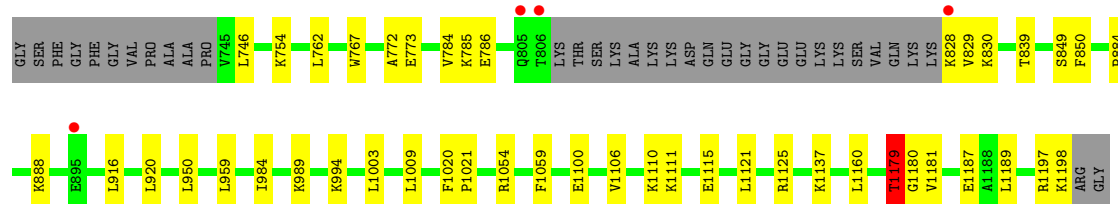
## • Molecule 2: Protein diaphanous homolog 1

## Chain H:



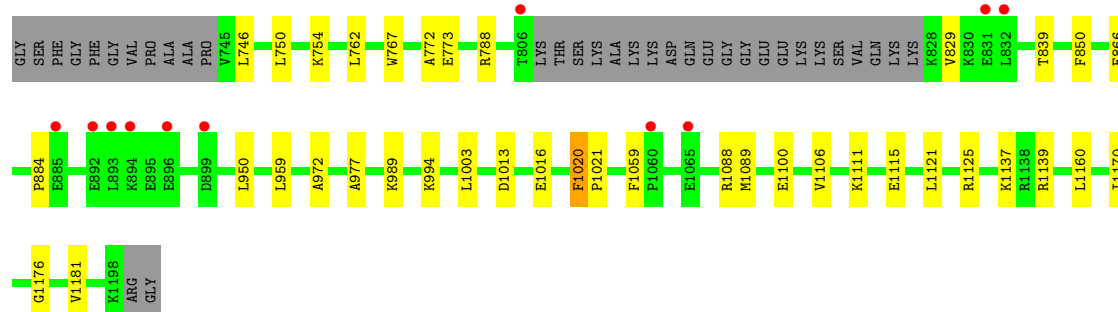
## • Molecule 2: Protein diaphanous homolog 1

## Chain G:



## • Molecule 2: Protein diaphanous homolog 1

## Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.76Å 206.83Å 131.06Å 90.00° 105.94° 90.00°	Depositor
Resolution (Å)	20.12 – 3.20 20.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.12-3.20) 99.1 (20.12-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.233 , 0.298 0.232 , 0.297	Depositor DCC
$R_{free}$ test set	3981 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 79565 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.36	0/2588	0.58	0/3483
1	B	0.37	0/2595	0.56	0/3493
1	C	0.37	0/2544	0.55	1/3425 (0.0%)
1	D	0.36	0/2605	0.55	1/3508 (0.0%)
2	E	0.37	0/3580	0.55	0/4799
2	F	0.36	0/3580	0.53	0/4799
2	G	0.36	0/3580	0.53	0/4799
2	H	0.38	0/3580	0.53	0/4799
All	All	0.37	0/24652	0.55	2/33105 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	371	LEU	CA-CB-CG	6.41	130.03	115.30
1	D	371	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2552	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2559	0	0	8	0
1	C	2508	0	0	7	0
1	D	2568	0	0	6	0
2	E	3525	0	0	8	0
2	F	3525	0	0	2	0
2	G	3525	0	0	3	0
2	H	3525	0	0	5	0
3	A	8	0	0	0	0
3	B	9	0	0	0	0
3	C	6	0	0	0	0
3	D	8	0	0	1	0
3	E	5	0	0	0	0
3	F	2	0	0	0	0
3	G	6	0	0	0	0
3	H	4	0	0	0	0
All	All	24335	0	0	39	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:411:VAL:CG2	1:D:411:VAL:O	2.45	0.65
1:B:388:ILE:CG1	1:C:409:LEU:CD1	2.75	0.65
2:E:1033:VAL:O	2:E:1115:GLU:CG	2.46	0.63
1:D:446:ARG:O	1:D:447:HIS:CB	2.46	0.61
2:E:784:VAL:C	2:E:786:GLU:N	2.54	0.61
1:A:411:VAL:O	1:A:411:VAL:CG2	2.49	0.60
1:B:200:TYR:C	1:B:202:SER:N	2.56	0.59
2:E:828:LYS:N	2:E:829:VAL:CA	2.68	0.57
1:B:411:VAL:O	1:B:411:VAL:CG2	2.54	0.54
2:H:950:LEU:CD1	2:H:1105:PHE:CE1	2.91	0.54
1:D:450:ILE:O	1:D:451:ASP:O	2.26	0.53
2:G:784:VAL:C	2:G:786:GLU:N	2.63	0.51
2:G:1179:THR:O	2:G:1181:VAL:N	2.46	0.48
2:F:1020:PHE:N	2:F:1021:PRO:CD	2.77	0.48
1:A:440:ASP:OD2	1:D:412:ARG:NH2	2.47	0.47
1:B:200:TYR:O	1:B:202:SER:N	2.48	0.47
1:B:413:ASN:OD1	1:B:418:ARG:NH2	2.49	0.46
1:C:411:VAL:O	1:C:411:VAL:CG2	2.63	0.46
2:E:786:GLU:O	2:E:788:ARG:N	2.48	0.46
1:A:248:ILE:CD1	1:A:301:LEU:CA	2.93	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:784:VAL:C	2:H:786:GLU:N	2.68	0.46
1:B:412:ARG:NH2	1:C:440:ASP:OD2	2.49	0.45
2:G:1020:PHE:N	2:G:1021:PRO:CD	2.80	0.45
1:B:446:ARG:CG	1:B:446:ARG:NH1	2.80	0.45
1:B:440:ASP:OD1	1:C:412:ARG:NH2	2.51	0.43
1:C:445:CYS:SG	1:C:446:ARG:N	2.92	0.43
1:A:297:THR:O	1:A:302:LYS:NZ	2.51	0.43
1:A:412:ARG:NH1	1:D:440:ASP:OD1	2.52	0.43
2:E:974:SER:O	2:E:975:ARG:C	2.56	0.42
2:E:786:GLU:C	2:E:788:ARG:N	2.72	0.42
2:E:1020:PHE:N	2:E:1021:PRO:CD	2.83	0.42
1:C:211:CYS:O	1:C:215:PHE:N	2.54	0.41
2:H:794:LEU:O	2:H:798:LEU:N	2.53	0.41
2:H:1076:PHE:O	2:H:1080:ALA:N	2.54	0.41
1:D:299:ILE:N	3:D:16:HOH:O	2.54	0.41
2:F:1088:ARG:NH1	2:F:1088:ARG:CG	2.84	0.41
1:C:410:LEU:O	1:C:411:VAL:C	2.59	0.40
2:E:953:SER:OG	2:E:1023:GLU:OE1	2.39	0.40
2:H:1197:ARG:O	2:H:1198:LYS:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/330 (95%)	299 (96%)	13 (4%)	1 (0%)	50	91
1	B	314/330 (95%)	296 (94%)	15 (5%)	3 (1%)	22	74
1	C	307/330 (93%)	289 (94%)	14 (5%)	4 (1%)	18	68
1	D	317/330 (96%)	296 (93%)	16 (5%)	5 (2%)	14	63
2	E	429/467 (92%)	390 (91%)	26 (6%)	13 (3%)	7	42
2	F	429/467 (92%)	387 (90%)	33 (8%)	9 (2%)	11	55
2	G	429/467 (92%)	389 (91%)	31 (7%)	9 (2%)	11	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	429/467 (92%)	384 (90%)	37 (9%)	8 (2%)	12	59
All	All	2967/3188 (93%)	2730 (92%)	185 (6%)	52 (2%)	13	60

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLU
1	C	264	GLU
1	D	447	HIS
1	D	451	ASP
2	E	975	ARG
2	E	1181	VAL
2	H	829	VAL
2	G	772	ALA
2	G	1180	GLY
2	F	772	ALA
2	F	829	VAL
2	F	1181	VAL
1	B	201	ASP
1	D	297	THR
2	E	772	ALA
2	E	787	ASP
2	H	1181	VAL
2	G	829	VAL
2	G	1179	THR
1	C	295	SER
1	D	264	GLU
2	E	785	LYS
2	E	977	ALA
2	E	1062	ALA
2	E	1173	ASN
2	E	1197	ARG
2	H	972	ALA
2	G	785	LYS
2	F	972	ALA
2	F	977	ALA
1	C	297	THR
2	E	746	LEU
2	E	972	ALA
2	E	1106	VAL
2	G	746	LEU
2	G	830	LYS

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Mol	Chain	Res	Type
2	F	746	LEU
2	F	1106	VAL
1	B	194	GLU
2	E	1174	ALA
2	H	830	LYS
2	H	884	PRO
1	B	264	GLU
2	H	746	LEU
2	F	1176	GLY
1	D	411	VAL
2	H	1106	VAL
2	H	1180	GLY
2	G	1106	VAL
2	G	884	PRO
1	C	261	PRO
2	F	884	PRO

### 5.3.2 Protein sidechains ⓘ

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	287/299 (96%)	264 (92%)	23 (8%)	17	57
1	B	288/299 (96%)	270 (94%)	18 (6%)	25	69
1	C	282/299 (94%)	264 (94%)	18 (6%)	25	69
1	D	289/299 (97%)	262 (91%)	27 (9%)	13	46
2	E	391/416 (94%)	351 (90%)	40 (10%)	11	40
2	F	391/416 (94%)	363 (93%)	28 (7%)	21	63
2	G	391/416 (94%)	358 (92%)	33 (8%)	16	53
2	H	391/416 (94%)	358 (92%)	33 (8%)	16	53
All	All	2710/2860 (95%)	2490 (92%)	220 (8%)	17	56

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LYS

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Mol	Chain	Res	Type
1	A	201	ASP
1	A	203	ARG
1	A	223	LYS
1	A	225	MET
1	A	235	LEU
1	A	252	LYS
1	A	260	LEU
1	A	277	ARG
1	A	283	VAL
1	A	299	ILE
1	A	318	GLU
1	A	329	LEU
1	A	332	LEU
1	A	334	LEU
1	A	345	GLU
1	A	367	LEU
1	A	391	THR
1	A	412	ARG
1	A	427	GLU
1	A	434	LEU
1	A	446	ARG
1	A	452	ILE
1	B	201	ASP
1	B	213	LYS
1	B	225	MET
1	B	230	GLU
1	B	243	VAL
1	B	269	ARG
1	B	277	ARG
1	B	322	ARG
1	B	325	ILE
1	B	329	LEU
1	B	334	LEU
1	B	367	LEU
1	B	374	ILE
1	B	392	VAL
1	B	408	LEU
1	B	409	LEU
1	B	427	GLU
1	B	436	LYS
1	C	149	ASP
1	C	169	SER

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Mol	Chain	Res	Type
1	C	225	MET
1	C	230	GLU
1	C	275	THR
1	C	329	LEU
1	C	332	LEU
1	C	334	LEU
1	C	367	LEU
1	C	377	GLU
1	C	391	THR
1	C	427	GLU
1	C	434	LEU
1	C	436	LYS
1	C	446	ARG
1	C	447	HIS
1	C	449	GLN
1	C	450	ILE
1	D	154	SER
1	D	187	LYS
1	D	191	ASP
1	D	200	TYR
1	D	223	LYS
1	D	225	MET
1	D	248	ILE
1	D	269	ARG
1	D	281	ASP
1	D	312	LEU
1	D	329	LEU
1	D	332	LEU
1	D	334	LEU
1	D	345	GLU
1	D	367	LEU
1	D	371	LEU
1	D	377	GLU
1	D	392	VAL
1	D	408	LEU
1	D	409	LEU
1	D	427	GLU
1	D	428	CYS
1	D	434	LEU
1	D	436	LYS
1	D	446	ARG
1	D	447	HIS

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Mol	Chain	Res	Type
1	D	449	GLN
2	E	746	LEU
2	E	753	LYS
2	E	754	LYS
2	E	762	LEU
2	E	767	TRP
2	E	773	GLU
2	E	779	CYS
2	E	787	ASP
2	E	829	VAL
2	E	839	THR
2	E	883	GLU
2	E	916	LEU
2	E	920	LEU
2	E	936	ILE
2	E	950	LEU
2	E	954	GLU
2	E	959	LEU
2	E	976	ASN
2	E	984	ILE
2	E	989	LYS
2	E	994	LYS
2	E	1002	LEU
2	E	1003	LEU
2	E	1006	LEU
2	E	1020	PHE
2	E	1059	PHE
2	E	1087	LEU
2	E	1100	GLU
2	E	1110	LYS
2	E	1111	LYS
2	E	1115	GLU
2	E	1121	LEU
2	E	1125	ARG
2	E	1132	VAL
2	E	1137	LYS
2	E	1160	LEU
2	E	1169	LEU
2	E	1170	ILE
2	E	1189	LEU
2	E	1198	LYS
2	H	746	LEU

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Mol	Chain	Res	Type
2	H	754	LYS
2	H	762	LEU
2	H	767	TRP
2	H	771	VAL
2	H	773	GLU
2	H	800	LEU
2	H	828	LYS
2	H	916	LEU
2	H	921	ASN
2	H	950	LEU
2	H	959	LEU
2	H	984	ILE
2	H	989	LYS
2	H	994	LYS
2	H	1000	MET
2	H	1002	LEU
2	H	1003	LEU
2	H	1016	GLU
2	H	1054	ARG
2	H	1059	PHE
2	H	1087	LEU
2	H	1100	GLU
2	H	1103	ASP
2	H	1110	LYS
2	H	1111	LYS
2	H	1115	GLU
2	H	1125	ARG
2	H	1137	LYS
2	H	1160	LEU
2	H	1171	ASP
2	H	1197	ARG
2	H	1198	LYS
2	G	754	LYS
2	G	762	LEU
2	G	767	TRP
2	G	773	GLU
2	G	828	LYS
2	G	839	THR
2	G	849	SER
2	G	850	PHE
2	G	888	LYS
2	G	916	LEU

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Mol	Chain	Res	Type
2	G	920	LEU
2	G	950	LEU
2	G	959	LEU
2	G	984	ILE
2	G	989	LYS
2	G	994	LYS
2	G	1003	LEU
2	G	1009	LEU
2	G	1054	ARG
2	G	1059	PHE
2	G	1100	GLU
2	G	1110	LYS
2	G	1111	LYS
2	G	1115	GLU
2	G	1121	LEU
2	G	1125	ARG
2	G	1137	LYS
2	G	1160	LEU
2	G	1179	THR
2	G	1187	GLU
2	G	1189	LEU
2	G	1197	ARG
2	G	1198	LYS
2	F	750	LEU
2	F	754	LYS
2	F	762	LEU
2	F	767	TRP
2	F	773	GLU
2	F	788	ARG
2	F	839	THR
2	F	850	PHE
2	F	866	GLU
2	F	950	LEU
2	F	959	LEU
2	F	989	LYS
2	F	994	LYS
2	F	1003	LEU
2	F	1013	ASP
2	F	1016	GLU
2	F	1020	PHE
2	F	1059	PHE
2	F	1089	MET

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Mol	Chain	Res	Type
2	F	1100	GLU
2	F	1111	LYS
2	F	1115	GLU
2	F	1121	LEU
2	F	1125	ARG
2	F	1137	LYS
2	F	1139	ARG
2	F	1160	LEU
2	F	1170	ILE

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9	
1	A	317/330 (96%)	-0.34	0	100	100	30, 75, 117, 149	2 (0%)
1	B	318/330 (96%)	-0.34	0	100	100	38, 79, 131, 157	2 (0%)
1	C	311/330 (94%)	-0.34	0	100	100	30, 80, 129, 213	2 (0%)
1	D	319/330 (96%)	-0.16	1 (0%)	91	58	31, 112, 166, 198	2 (0%)
2	E	433/467 (92%)	-0.20	1 (0%)	93	66	47, 94, 144, 177	0
2	F	433/467 (92%)	0.08	11 (2%)	54	12	61, 133, 211, 256	0
2	G	433/467 (92%)	-0.00	4 (0%)	81	32	68, 127, 172, 209	0
2	H	433/467 (92%)	-0.11	3 (0%)	84	38	40, 110, 166, 200	0
All	All	2997/3188 (94%)	-0.16	20 (0%)	84	38	30, 102, 173, 256	8 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	831	GLU	3.7
2	F	899	ASP	3.6
2	F	1065	GLU	3.6
2	F	806	THR	2.8
2	H	1175	GLU	2.7
2	H	1174	ALA	2.7
2	G	805	GLN	2.4
2	G	895	GLU	2.4
2	F	832	LEU	2.3
2	F	894	LYS	2.3
2	F	1060	PRO	2.2
2	E	828	LYS	2.2
2	F	892	GLU	2.2
2	H	1176	GLY	2.2
2	G	806	THR	2.1
2	F	885	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	196	THR	2.1
2	G	828	LYS	2.0
2	F	896	GLU	2.0
2	F	893	LEU	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.