Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:14 PM GMT

PDB ID	:	4KZG
Title	:	Crystal structure of zebrafish MO25
Authors	:	Zhang, Z.Z.; Shi, Z.B.; Zhang, M.
Deposited on	:	2013-05-30
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 ⓘ symbol.

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

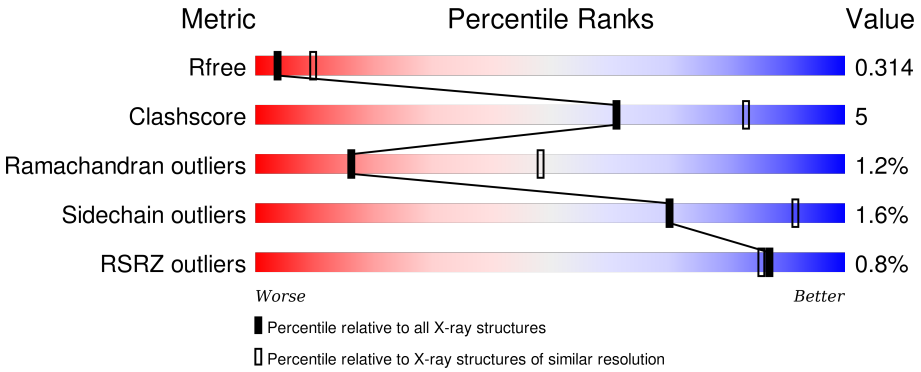
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	327	% 80% 15% • •
1	B	327	% 86% 10% •
1	C	327	% 86% 11% • •
1	D	327	81% 14% • 5%
1	E	327	81% 15% •

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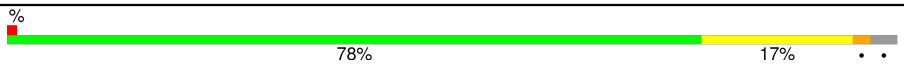
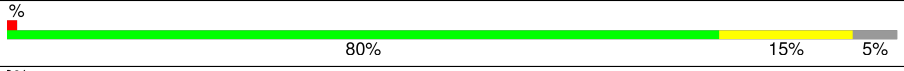
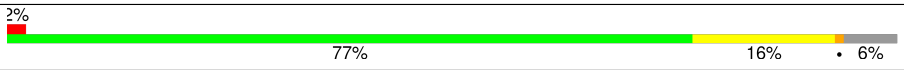
Mol	Chain	Length	Quality of chain
1	F	327	
1	G	327	
1	H	327	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20074 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 Zgc:86716.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2526	1620	412	482	12			
1	B	314	Total	C	N	O	S	0	0	0
			2517	1618	414	474	11			
1	C	318	Total	C	N	O	S	0	0	0
			2540	1628	418	482	12			
1	D	312	Total	C	N	O	S	0	0	0
			2489	1597	409	473	10			
1	E	314	Total	C	N	O	S	0	0	0
			2520	1615	416	478	11			
1	F	316	Total	C	N	O	S	0	1	0
			2555	1643	421	480	11			
1	G	312	Total	C	N	O	S	0	0	0
			2490	1598	414	467	11			
1	H	307	Total	C	N	O	S	0	0	0
			2398	1539	389	460	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2
A	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
A	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
A	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2
B	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2
B	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
B	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
B	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2
C	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2
C	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
C	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
C	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2
D	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
D	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
D	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2
E	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2
E	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
E	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
E	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2
F	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2
F	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
F	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
F	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2
G	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2
G	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
G	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
G	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2
H	8	GLY	-	EXPRESSION TAG	UNP Q6IQL2
H	9	ALA	-	EXPRESSION TAG	UNP Q6IQL2
H	10	MET	-	EXPRESSION TAG	UNP Q6IQL2
H	11	ALA	-	EXPRESSION TAG	UNP Q6IQL2

- Molecule 2 is water.

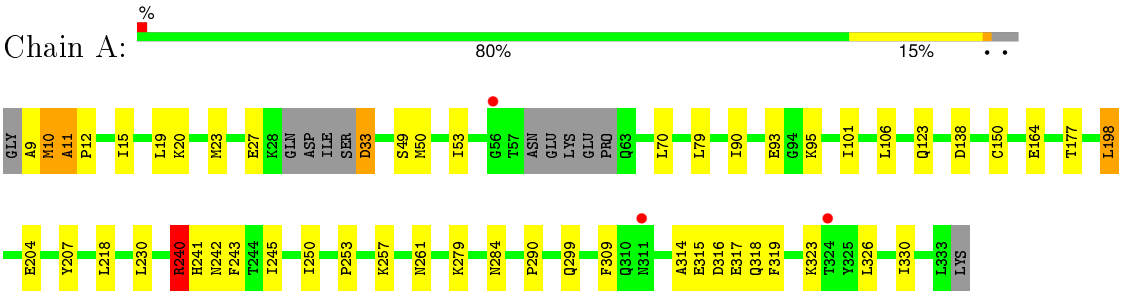
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0
2	B	6	Total O 6 6	0	0
2	C	10	Total O 10 10	0	0
2	E	4	Total O 4 4	0	0
2	F	7	Total O 7 7	0	0
2	G	3	Total O 3 3	0	0
2	H	1	Total O 1 1	0	0

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.

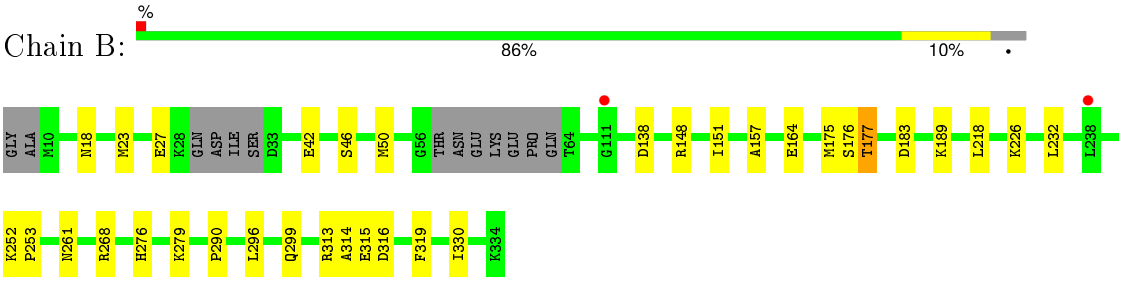
- Molecule 1: Zgc:86716

Chain A:



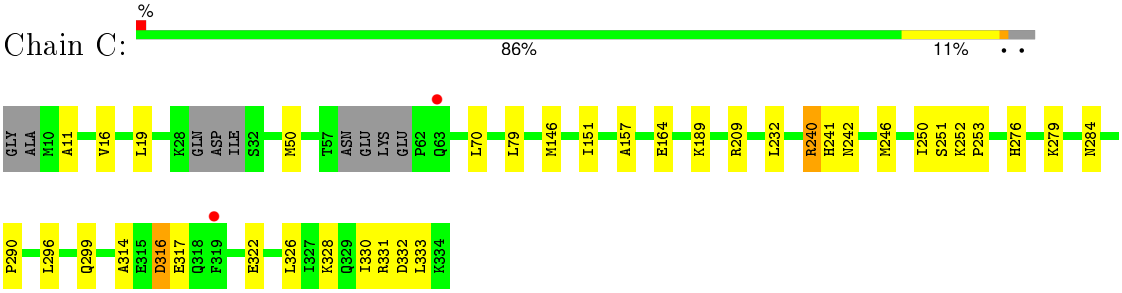
- Molecule 1: Zgc:86716

Chain B:



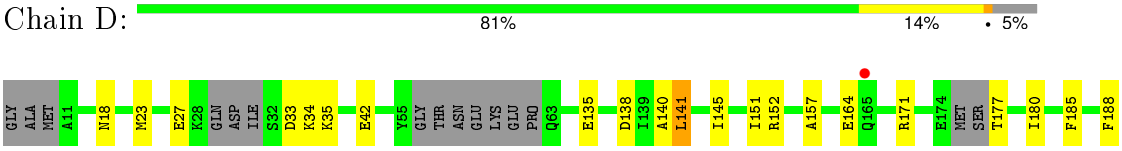
- Molecule 1: Zgc:86716

Chain C:



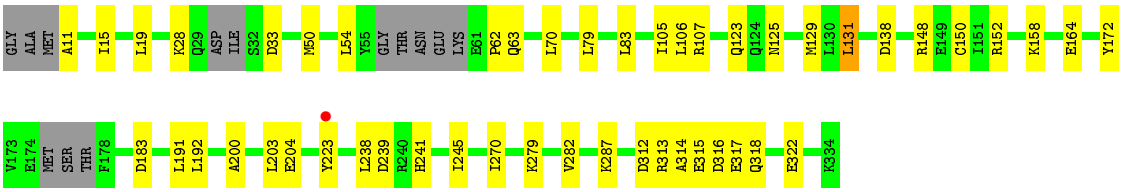
- Molecule 1: Zgc:86716

Chain D:



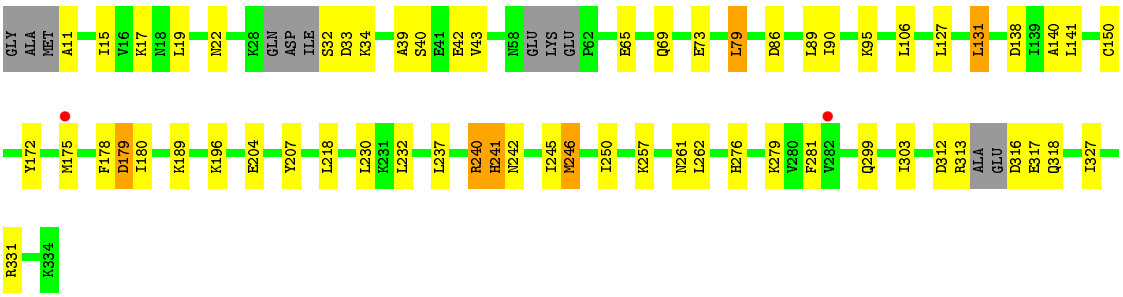
• Molecule 1: Zgc:86716

Chain E:



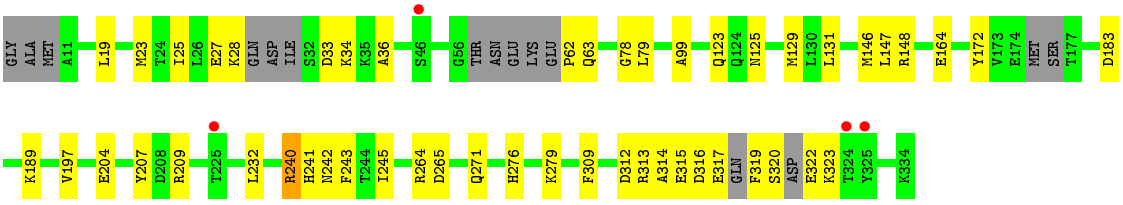
• Molecule 1: Zgc:86716

Chain F:



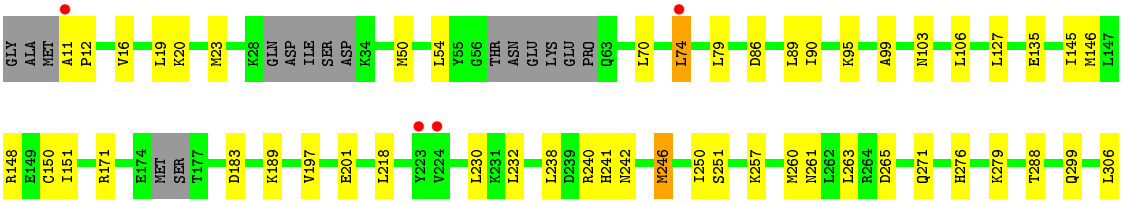
• Molecule 1: Zgc:86716

Chain G:



• Molecule 1: Zgc:86716

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	156.66Å 156.66Å 221.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.96 – 2.90 49.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.96-2.90) 89.0 (49.96-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.288 , 0.327 0.276 , 0.314	Depositor DCC
R_{free} test set	1758 reflections (2.83%)	DCC
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , -6.9	EDS
Estimated twinning fraction	0.087 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	32 of 69875 reflections (0.046%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	20074	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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 52.93 % 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 4.5341e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/2568	0.47	1/3465 (0.0%)
1	B	0.26	0/2559	0.46	0/3451
1	C	0.25	0/2583	0.47	0/3486
1	D	0.25	0/2529	0.47	0/3417
1	E	0.25	0/2561	0.48	0/3456
1	F	0.25	0/2598	0.49	0/3500
1	G	0.25	0/2529	0.48	0/3406
1	H	0.25	0/2437	0.46	0/3293
All	All	0.25	0/20364	0.47	1/27474 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	LEU	CA-CB-CG	5.08	127.00	115.30

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	2526	0	2481	34	0
1	B	2517	0	2495	23	0
1	C	2540	0	2501	19	0
1	D	2489	0	2444	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2520	0	2485	30	0
1	F	2555	0	2541	35	0
1	G	2490	0	2461	30	0
1	H	2398	0	2289	30	0
2	A	8	0	0	0	0
2	B	6	0	0	0	0
2	C	10	0	0	0	0
2	E	4	0	0	0	0
2	F	7	0	0	1	0
2	G	3	0	0	1	0
2	H	1	0	0	0	0
All	All	20074	0	19697	217	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 5.

All (217) 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:E:107:ARG:HH21	1:E:152:ARG:HE	1.18	0.90
1:D:204:GLU:HA	1:D:245:ILE:HD11	1.58	0.85
1:F:22:ASN:ND2	1:F:39:ALA:O	2.16	0.78
1:D:316:ASP:O	1:D:318:GLN:N	2.15	0.78
1:G:164:GLU:OE1	1:G:209:ARG:NH1	2.18	0.76
1:A:204:GLU:HA	1:A:245:ILE:HD11	1.67	0.76
1:B:177:THR:HG22	1:F:178[B]:PHE:HB3	1.71	0.73
1:F:316:ASP:O	1:F:318:GLN:N	2.22	0.73
1:B:164:GLU:H	1:G:123:GLN:HE22	1.37	0.71
1:C:328:LYS:NZ	1:C:332:ASP:OD2	2.22	0.71
1:F:303:ILE:HG13	1:F:327:ILE:HG23	1.74	0.70
1:D:314:ALA:O	1:D:316:ASP:N	2.20	0.70
1:E:314:ALA:O	1:E:316:ASP:N	2.25	0.69
1:E:316:ASP:O	1:E:318:GLN:N	2.22	0.69
1:H:306:LEU:HB2	1:H:327:ILE:HD11	1.75	0.69
1:C:164:GLU:OE1	1:C:209:ARG:NH1	2.20	0.69
1:E:107:ARG:NH2	1:E:152:ARG:HE	1.91	0.68
1:F:22:ASN:ND2	1:F:42:GLU:HB2	2.09	0.68
1:G:25:ILE:HA	1:G:28:LYS:HE2	1.76	0.68
1:G:320:SER:O	1:G:322:GLU:N	2.27	0.67
1:A:314:ALA:O	1:A:316:ASP:N	2.26	0.67
1:A:316:ASP:O	1:A:318:GLN:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:GLU:HA	1:G:320:SER:HB2	1.77	0.65
1:D:151:ILE:HD12	1:D:157:ALA:HA	1.78	0.65
1:B:314:ALA:O	1:B:316:ASP:N	2.26	0.65
1:C:279:LYS:NZ	1:C:322:GLU:OE2	2.30	0.64
1:A:240:ARG:O	1:A:242:ASN:N	2.30	0.64
1:D:279:LYS:NZ	1:D:322:GLU:OE2	2.26	0.64
1:B:151:ILE:HD12	1:B:157:ALA:HA	1.80	0.64
1:G:312:ASP:OD1	1:G:313:ARG:N	2.31	0.63
1:D:207:TYR:HD2	1:D:245:ILE:HD12	1.65	0.61
1:F:218:LEU:HD22	1:F:230:LEU:HD13	1.82	0.61
1:B:177:THR:HG22	1:F:178[A]:PHE:HB2	1.82	0.60
1:G:316:ASP:HB3	1:G:319:PHE:HB3	1.83	0.60
1:A:33:ASP:OD1	1:A:33:ASP:N	2.35	0.60
1:H:197:VAL:O	1:H:201:GLU:HG3	2.01	0.60
1:D:299:GLN:HG3	1:D:330:ILE:HG22	1.83	0.60
1:A:314:ALA:C	1:A:316:ASP:H	2.06	0.60
1:A:316:ASP:HB3	1:A:319:PHE:HB3	1.82	0.60
1:C:151:ILE:HD12	1:C:157:ALA:HA	1.83	0.59
1:D:265:ASP:O	1:D:271:GLN:NE2	2.36	0.58
1:E:314:ALA:C	1:E:316:ASP:H	2.05	0.58
1:D:164:GLU:OE1	1:D:209:ARG:NH1	2.27	0.58
1:G:279:LYS:NZ	1:G:322:GLU:OE2	2.35	0.58
1:A:240:ARG:O	1:A:243:PHE:N	2.37	0.58
1:G:309:PHE:O	1:G:323:LYS:NZ	2.30	0.58
1:F:106:LEU:HD21	1:F:150:CYS:HA	1.86	0.58
1:A:253:PRO:HG3	1:A:290:PRO:HB2	1.86	0.57
1:B:164:GLU:H	1:G:123:GLN:NE2	2.01	0.57
1:A:20:LYS:HG2	1:A:79:LEU:HD13	1.86	0.57
1:C:276:HIS:HA	1:C:279:LYS:HD3	1.85	0.57
1:D:316:ASP:HB3	1:D:319:PHE:HB3	1.87	0.57
1:F:204:GLU:HA	1:F:245:ILE:HD11	1.85	0.57
1:E:107:ARG:HH21	1:E:152:ARG:NE	1.98	0.56
1:D:299:GLN:NE2	1:D:330:ILE:O	2.38	0.56
1:F:207:TYR:HD2	1:F:245:ILE:HD12	1.70	0.56
1:C:330:ILE:HA	1:C:333:LEU:HD13	1.86	0.56
1:B:314:ALA:C	1:B:316:ASP:H	2.08	0.56
1:A:207:TYR:HD2	1:A:245:ILE:HD12	1.70	0.56
1:F:240:ARG:O	1:F:242:ASN:N	2.38	0.56
1:A:23:MET:O	1:A:27:GLU:HG3	2.06	0.56
1:F:303:ILE:HD12	1:F:331:ARG:HG3	1.88	0.55
1:G:240:ARG:O	1:G:242:ASN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:HE22	1:E:164:GLU:H	1.54	0.55
1:A:90:ILE:O	1:A:95:LYS:NZ	2.27	0.55
1:D:18:ASN:HD21	1:D:42:GLU:HG3	1.72	0.54
1:G:123:GLN:NE2	2:G:401:HOH:O	2.18	0.54
1:B:18:ASN:HD21	1:B:42:GLU:HG3	1.72	0.54
1:B:316:ASP:HB3	1:B:319:PHE:HB3	1.89	0.54
1:D:135:GLU:OE2	1:D:171:ARG:NH2	2.40	0.54
1:C:253:PRO:HG3	1:C:290:PRO:HB2	1.89	0.54
1:G:131:LEU:HD23	1:G:172:TYR:HE2	1.73	0.54
1:A:9:ALA:HA	1:A:10:MET:O	2.09	0.53
1:H:106:LEU:HD21	1:H:150:CYS:HA	1.91	0.53
1:E:106:LEU:HD21	1:E:150:CYS:HA	1.91	0.53
1:F:131:LEU:HD22	1:F:172:TYR:HE2	1.74	0.53
1:E:239:ASP:OD2	1:E:241:HIS:ND1	2.38	0.53
1:F:257:LYS:O	1:F:261:ASN:HB2	2.08	0.53
1:A:299:GLN:HG3	1:A:330:ILE:HG22	1.92	0.52
1:F:175:MET:HA	1:F:178[A]:PHE:HE1	1.73	0.52
1:E:50:MET:HG3	1:E:70:LEU:HD11	1.91	0.52
1:H:265:ASP:O	1:H:271:GLN:NE2	2.42	0.52
1:D:23:MET:O	1:D:27:GLU:HG3	2.10	0.52
1:G:19:LEU:HD23	1:G:79:LEU:HD21	1.90	0.52
1:F:230:LEU:HD21	1:F:262:LEU:HD13	1.91	0.51
1:E:11:ALA:O	1:E:15:ILE:HG13	2.11	0.51
1:B:23:MET:O	1:B:27:GLU:HG3	2.11	0.51
1:H:103:ASN:HD21	1:H:145:ILE:HG22	1.76	0.51
1:G:265:ASP:O	1:G:271:GLN:NE2	2.44	0.51
1:G:276:HIS:HA	1:G:279:LYS:HD3	1.93	0.51
1:H:189:LYS:HG3	1:H:232:LEU:HD13	1.93	0.50
1:F:90:ILE:O	1:F:95:LYS:HE3	2.10	0.50
1:H:240:ARG:HH11	1:H:241:HIS:H	1.60	0.50
1:F:73:GLU:OE1	2:F:406:HOH:O	2.20	0.50
1:C:50:MET:HG2	1:C:70:LEU:HD21	1.94	0.50
1:G:33:ASP:O	1:G:36:ALA:N	2.40	0.50
1:A:326:LEU:O	1:A:330:ILE:HG12	2.11	0.49
1:A:164:GLU:H	1:E:123:GLN:NE2	2.10	0.49
1:G:125:ASN:O	1:G:129:MET:HG2	2.12	0.49
1:A:164:GLU:H	1:E:123:GLN:HE22	1.60	0.49
1:C:316:ASP:O	1:C:317:GLU:HB2	2.13	0.49
1:E:131:LEU:HD22	1:E:172:TYR:HE2	1.77	0.49
1:F:86:ASP:HB3	1:F:89:LEU:HD12	1.94	0.48
1:G:314:ALA:O	1:G:316:ASP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:GLU:O	1:F:69:GLN:HG2	2.12	0.48
1:H:16:VAL:HG13	1:H:79:LEU:HD22	1.95	0.48
1:D:140:ALA:HB3	1:D:180:ILE:HD12	1.95	0.48
1:D:250:ILE:HA	1:D:281:PHE:CE2	2.48	0.48
1:E:19:LEU:HD23	1:E:79:LEU:HD21	1.95	0.48
1:C:326:LEU:O	1:C:330:ILE:HG13	2.13	0.48
1:B:177:THR:HA	1:F:178[A]:PHE:CD2	2.49	0.47
1:A:123:GLN:NE2	1:E:164:GLU:H	2.12	0.47
1:D:240:ARG:O	1:D:242:ASN:N	2.48	0.47
1:A:50:MET:HB3	1:A:101:ILE:HD13	1.97	0.47
1:F:32:SER:O	1:F:34:LYS:N	2.41	0.47
1:G:148:ARG:NH1	1:G:183:ASP:OD2	2.27	0.47
1:F:19:LEU:HD23	1:F:79:LEU:HD11	1.96	0.47
1:H:299:GLN:HG3	1:H:330:ILE:HG22	1.96	0.47
1:H:99:ALA:HA	1:H:146:MET:SD	2.55	0.47
1:H:148:ARG:NH1	1:H:183:ASP:OD1	2.29	0.47
1:F:312:ASP:OD1	1:F:313:ARG:N	2.48	0.46
1:C:240:ARG:O	1:C:242:ASN:N	2.48	0.46
1:H:135:GLU:OE2	1:H:171:ARG:NH2	2.49	0.46
1:C:189:LYS:HG3	1:C:232:LEU:HD13	1.97	0.46
1:F:138:ASP:OD1	1:F:138:ASP:N	2.44	0.46
1:H:90:ILE:O	1:H:95:LYS:HE3	2.15	0.46
1:F:276:HIS:HA	1:F:279:LYS:HE2	1.96	0.46
1:B:164:GLU:OE1	1:G:78:GLY:HA3	2.15	0.46
1:D:326:LEU:O	1:D:330:ILE:HG12	2.15	0.46
1:E:138:ASP:N	1:E:138:ASP:OD1	2.42	0.46
1:A:309:PHE:O	1:A:323:LYS:NZ	2.29	0.46
1:B:253:PRO:HG3	1:B:290:PRO:HB2	1.99	0.45
1:E:312:ASP:OD1	1:E:313:ARG:N	2.50	0.45
1:A:106:LEU:HD21	1:A:150:CYS:HA	1.98	0.45
1:H:70:LEU:O	1:H:74:LEU:HD22	2.17	0.45
1:E:203:LEU:HB3	1:E:245:ILE:HG12	1.97	0.45
1:D:138:ASP:N	1:D:138:ASP:OD1	2.48	0.45
1:E:279:LYS:NZ	1:E:322:GLU:OE2	2.50	0.45
1:H:86:ASP:HB3	1:H:89:LEU:HD12	1.98	0.45
1:E:148:ARG:HH12	1:E:183:ASP:CG	2.21	0.45
1:B:46:SER:O	1:B:50:MET:HB2	2.17	0.45
1:H:20:LYS:HE2	1:H:20:LYS:HB3	1.75	0.45
1:A:11:ALA:HA	1:A:12:PRO:HD3	1.84	0.44
1:F:11:ALA:O	1:F:15:ILE:HG13	2.17	0.44
1:G:207:TYR:HD2	1:G:245:ILE:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLN:HG3	1:C:330:ILE:HG22	1.98	0.44
1:A:138:ASP:OD1	1:A:138:ASP:N	2.50	0.44
1:A:19:LEU:HD23	1:A:79:LEU:HD21	1.99	0.44
1:F:40:SER:O	1:F:43:VAL:HG22	2.18	0.44
1:F:140:ALA:HB3	1:F:180:ILE:HD12	1.99	0.44
1:H:240:ARG:HG3	1:H:241:HIS:H	1.83	0.44
1:A:257:LYS:O	1:A:261:ASN:HB2	2.18	0.44
1:G:99:ALA:HA	1:G:146:MET:SD	2.58	0.44
1:E:200:ALA:O	1:E:204:GLU:HG3	2.18	0.44
1:F:189:LYS:HG3	1:F:232:LEU:HD13	1.99	0.44
1:G:314:ALA:C	1:G:316:ASP:H	2.20	0.44
1:H:148:ARG:HA	1:H:151:ILE:HG12	2.00	0.44
1:E:125:ASN:O	1:E:129:MET:HG2	2.18	0.43
1:G:62:PRO:HA	1:G:63:GLN:HA	1.72	0.43
1:H:251:SER:HB2	1:H:288:THR:HG21	2.00	0.43
1:D:314:ALA:C	1:D:316:ASP:H	2.14	0.43
1:A:218:LEU:HD22	1:A:230:LEU:HD13	1.99	0.43
1:H:276:HIS:HA	1:H:279:LYS:HD3	2.00	0.43
1:F:237:LEU:HD22	1:F:246:MET:HA	1.99	0.43
1:G:240:ARG:O	1:G:243:PHE:N	2.51	0.43
1:A:50:MET:HG3	1:A:70:LEU:HD11	2.01	0.43
1:E:223:TYR:HE1	1:E:270:ILE:HG12	1.83	0.43
1:F:250:ILE:HA	1:F:281:PHE:CE2	2.53	0.42
1:F:299:GLN:O	1:F:303:ILE:HG22	2.19	0.42
1:D:185:PHE:HA	1:D:188:PHE:HB3	2.02	0.42
1:C:16:VAL:HG13	1:C:79:LEU:HD22	2.01	0.42
1:B:189:LYS:HG3	1:B:232:LEU:HD13	2.00	0.42
1:B:299:GLN:HG3	1:B:330:ILE:HG22	2.02	0.42
1:E:79:LEU:HG	1:E:83:LEU:HG	2.00	0.42
1:H:257:LYS:O	1:H:261:ASN:HB2	2.18	0.42
1:D:231:LYS:O	1:D:235:GLU:HG3	2.19	0.42
1:H:279:LYS:NZ	1:H:322:GLU:OE2	2.38	0.42
1:D:33:ASP:O	1:D:35:LYS:N	2.52	0.42
1:E:282:VAL:O	1:E:287:LYS:NZ	2.35	0.42
1:C:252:LYS:HA	1:C:253:PRO:HD3	1.90	0.42
1:D:326:LEU:HA	1:D:326:LEU:HD23	1.91	0.42
1:F:246:MET:O	1:F:250:ILE:HG12	2.19	0.42
1:C:19:LEU:HD23	1:C:79:LEU:HD21	2.01	0.42
1:B:276:HIS:HA	1:B:279:LYS:HE2	2.02	0.42
1:A:15:ILE:HD12	1:A:53:ILE:HD11	2.01	0.42
1:H:240:ARG:C	1:H:242:ASN:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:PRO:HG3	1:D:290:PRO:HB2	2.02	0.41
1:H:238:LEU:HA	1:H:238:LEU:HD23	1.91	0.41
1:F:196:LYS:HB3	1:F:241:HIS:CG	2.54	0.41
1:B:218:LEU:O	1:B:226:LYS:HE3	2.20	0.41
1:C:250:ILE:HD12	1:C:284:ASN:HB2	2.02	0.41
1:E:50:MET:HG2	1:E:70:LEU:HD21	2.01	0.41
1:B:175:MET:HA	1:B:176:SER:HA	1.74	0.41
1:E:158:LYS:HE2	1:E:158:LYS:HB3	1.82	0.41
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.84	0.41
1:H:218:LEU:HD22	1:H:230:LEU:HD13	2.01	0.41
1:G:189:LYS:HG3	1:G:232:LEU:HD13	2.02	0.41
1:D:291:ILE:HA	1:D:291:ILE:HD13	1.92	0.41
1:G:23:MET:O	1:G:27:GLU:HG3	2.20	0.41
1:H:260:MET:O	1:H:263:LEU:HB2	2.20	0.41
1:E:314:ALA:C	1:E:316:ASP:N	2.74	0.41
1:G:204:GLU:HA	1:G:245:ILE:HD11	2.02	0.41
1:B:268:ARG:NH2	1:B:313:ARG:HB2	2.36	0.41
1:A:250:ILE:HD12	1:A:284:ASN:HB2	2.02	0.41
1:H:11:ALA:HA	1:H:12:PRO:HD3	1.92	0.41
1:B:279:LYS:HE2	1:B:279:LYS:HB3	1.85	0.41
1:D:141:LEU:O	1:D:145:ILE:HG13	2.21	0.41
1:B:148:ARG:NH1	1:B:183:ASP:OD2	2.42	0.41
1:H:246:MET:O	1:H:250:ILE:HG12	2.21	0.41
1:B:164:GLU:N	1:G:123:GLN:HE22	2.12	0.40
1:A:49:SER:O	1:A:53:ILE:HG13	2.20	0.40
1:E:54:LEU:HD21	1:E:105:ILE:HD11	2.02	0.40
1:C:296:LEU:HD21	1:C:333:LEU:HB3	2.02	0.40
1:A:93:GLU:OE1	1:C:331:ARG:NH2	2.53	0.40
1:H:19:LEU:O	1:H:23:MET:HG2	2.21	0.40
1:H:50:MET:O	1:H:54:LEU:HG	2.22	0.40
1:D:207:TYR:CD2	1:D:245:ILE:HD12	2.51	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	310/327 (95%)	293 (94%)	11 (4%)	6 (2%)	10	35
1	B	308/327 (94%)	299 (97%)	8 (3%)	1 (0%)	46	79
1	C	312/327 (95%)	298 (96%)	10 (3%)	4 (1%)	15	46
1	D	304/327 (93%)	290 (95%)	9 (3%)	5 (2%)	12	40
1	E	306/327 (94%)	292 (95%)	9 (3%)	5 (2%)	12	40
1	F	309/327 (94%)	295 (96%)	9 (3%)	5 (2%)	12	40
1	G	300/327 (92%)	286 (95%)	10 (3%)	4 (1%)	15	46
1	H	297/327 (91%)	287 (97%)	10 (3%)	0	100	100
All	All	2446/2616 (94%)	2340 (96%)	76 (3%)	30 (1%)	16	48

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	A	317	GLU
1	C	241	HIS
1	D	241	HIS
1	D	315	GLU
1	D	317	GLU
1	E	317	GLU
1	F	241	HIS
1	F	317	GLU
1	G	241	HIS
1	A	315	GLU
1	B	315	GLU
1	E	62	PRO
1	E	315	GLU
1	F	179	ASP
1	C	240	ARG
1	C	314	ALA
1	D	34	LYS
1	D	240	ARG
1	E	28	LYS
1	E	63	GLN
1	F	240	ARG
1	G	34	LYS
1	G	240	ARG

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Mol	Chain	Res	Type
1	G	315	GLU
1	A	10	MET
1	A	240	ARG
1	F	33	ASP
1	A	11	ALA
1	C	11	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	273/300 (91%)	269 (98%)	4 (2%)	72	92
1	B	273/300 (91%)	268 (98%)	5 (2%)	66	90
1	C	276/300 (92%)	272 (99%)	4 (1%)	74	93
1	D	269/300 (90%)	265 (98%)	4 (2%)	72	92
1	E	274/300 (91%)	269 (98%)	5 (2%)	66	90
1	F	280/300 (93%)	273 (98%)	7 (2%)	55	85
1	G	268/300 (89%)	265 (99%)	3 (1%)	80	95
1	H	249/300 (83%)	246 (99%)	3 (1%)	78	94
All	All	2162/2400 (90%)	2127 (98%)	35 (2%)	70	91

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	177	THR
1	A	198	LEU
1	A	240	ARG
1	B	138	ASP
1	B	177	THR
1	B	252	LYS
1	B	261	ASN
1	B	296	LEU

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Mol	Chain	Res	Type
1	C	146	MET
1	C	246	MET
1	C	251	SER
1	C	316	ASP
1	D	141	LEU
1	D	152	ARG
1	D	177	THR
1	D	315	GLU
1	E	33	ASP
1	E	131	LEU
1	E	191	LEU
1	E	192	LEU
1	E	238	LEU
1	F	17	LYS
1	F	79	LEU
1	F	127	LEU
1	F	131	LEU
1	F	141	LEU
1	F	179	ASP
1	F	246	MET
1	G	147	LEU
1	G	197	VAL
1	G	264	ARG
1	H	74	LEU
1	H	127	LEU
1	H	246	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	B	125	ASN
1	E	123	GLN
1	F	22	ASN
1	G	123	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	316/327 (96%)	-0.15	3 (0%)	85	84	9, 23, 49, 63	0
1	B	314/327 (96%)	-0.22	2 (0%)	90	89	7, 23, 39, 62	0
1	C	318/327 (97%)	-0.19	2 (0%)	90	89	10, 23, 49, 70	0
1	D	312/327 (95%)	-0.16	1 (0%)	94	94	11, 27, 50, 74	0
1	E	314/327 (96%)	-0.14	1 (0%)	94	94	10, 24, 53, 93	0
1	F	316/327 (96%)	-0.08	2 (0%)	90	89	11, 27, 51, 62	0
1	G	312/327 (95%)	-0.02	4 (1%)	79	78	6, 27, 53, 81	0
1	H	307/327 (93%)	0.05	6 (1%)	68	64	12, 37, 58, 70	0
All	All	2509/2616 (95%)	-0.11	21 (0%)	87	86	6, 26, 52, 93	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	224	VAL	3.4
1	G	225	THR	3.0
1	H	326	LEU	2.9
1	G	324	THR	2.6
1	C	319	PHE	2.5
1	E	223	TYR	2.3
1	B	238	LEU	2.3
1	H	223	TYR	2.3
1	H	74	LEU	2.3
1	G	46	SER	2.3
1	B	111	GLY	2.3
1	F	175	MET	2.2
1	A	311	ASN	2.1
1	G	325	TYR	2.1
1	A	324	THR	2.1
1	F	282	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	11	ALA	2.1
1	D	165	GLN	2.1
1	A	56	GLY	2.0
1	H	322	GLU	2.0
1	C	63	GLN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.