



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:11 am GMT

PDB ID : 3VTI  
Title : Crystal structure of HypE-HypF complex  
Authors : Shomura, Y.; Higuchi, Y.  
Deposited on : 2012-05-30  
Resolution : 2.56 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](mailto: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.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

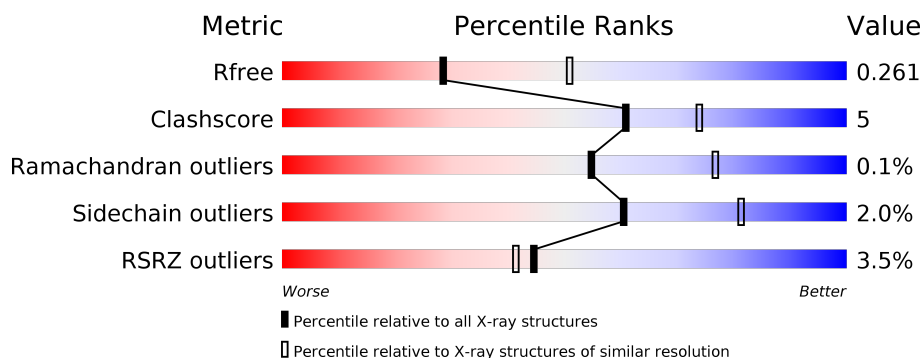
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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))
$R_{free}$	100719	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

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. 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  $\leq 5\%$ . 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	761	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	761	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>•</div> </div> </div>
2	C	314	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>•</div> </div> </div>
2	D	314	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	D	401	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16939 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 Hydrogenase maturation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	744	Total	C	N	O	S	0	0	0
			5964	3812	1013	1108	31			
1	B	744	Total	C	N	O	S	0	0	0
			5964	3812	1013	1108	31			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	SER	-	EXPRESSION TAG	UNP Q8RDB0
A	753	ALA	-	EXPRESSION TAG	UNP Q8RDB0
A	754	TRP	-	EXPRESSION TAG	UNP Q8RDB0
A	755	SER	-	EXPRESSION TAG	UNP Q8RDB0
A	756	HIS	-	EXPRESSION TAG	UNP Q8RDB0
A	757	PRO	-	EXPRESSION TAG	UNP Q8RDB0
A	758	GLN	-	EXPRESSION TAG	UNP Q8RDB0
A	759	PHE	-	EXPRESSION TAG	UNP Q8RDB0
A	760	GLU	-	EXPRESSION TAG	UNP Q8RDB0
A	761	LYS	-	EXPRESSION TAG	UNP Q8RDB0
B	752	SER	-	EXPRESSION TAG	UNP Q8RDB0
B	753	ALA	-	EXPRESSION TAG	UNP Q8RDB0
B	754	TRP	-	EXPRESSION TAG	UNP Q8RDB0
B	755	SER	-	EXPRESSION TAG	UNP Q8RDB0
B	756	HIS	-	EXPRESSION TAG	UNP Q8RDB0
B	757	PRO	-	EXPRESSION TAG	UNP Q8RDB0
B	758	GLN	-	EXPRESSION TAG	UNP Q8RDB0
B	759	PHE	-	EXPRESSION TAG	UNP Q8RDB0
B	760	GLU	-	EXPRESSION TAG	UNP Q8RDB0
B	761	LYS	-	EXPRESSION TAG	UNP Q8RDB0

- Molecule 2 is a protein called Hydrogenase maturation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	305	Total	C	N	O	S	0	0	0
			2305	1473	373	448	11			
2	D	305	Total	C	N	O	S	0	0	0
			2305	1473	373	448	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	GLY	-	EXPRESSION TAG	UNP Q8RDA7
C	39	ALA	-	EXPRESSION TAG	UNP Q8RDA7
D	38	GLY	-	EXPRESSION TAG	UNP Q8RDA7
D	39	ALA	-	EXPRESSION TAG	UNP Q8RDA7

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	177	Total	O	0	0
			177	177		

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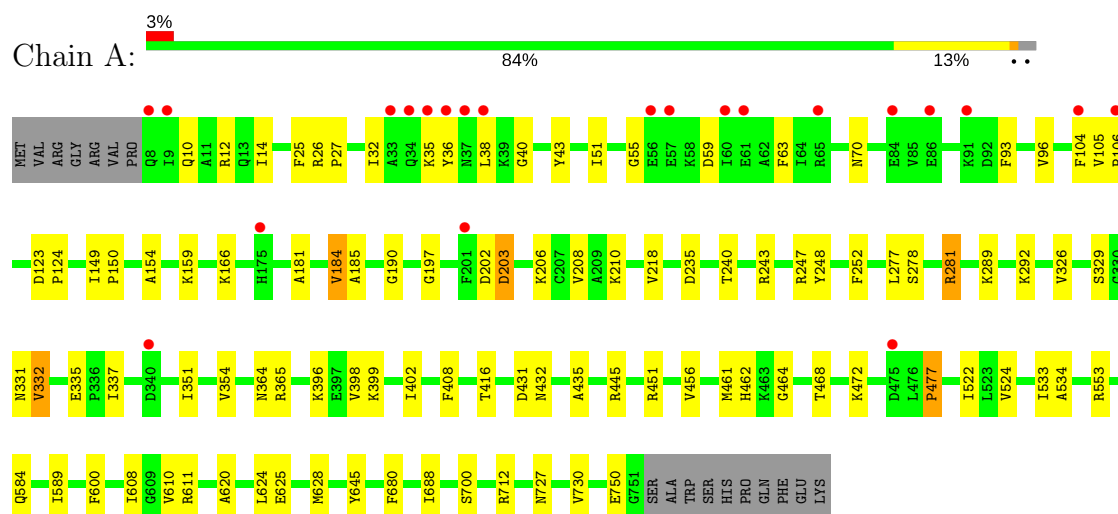
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	113	Total 113	O 113	0	0
6	C	58	Total 58	O 58	0	0
6	D	45	Total 45	O 45	0	0

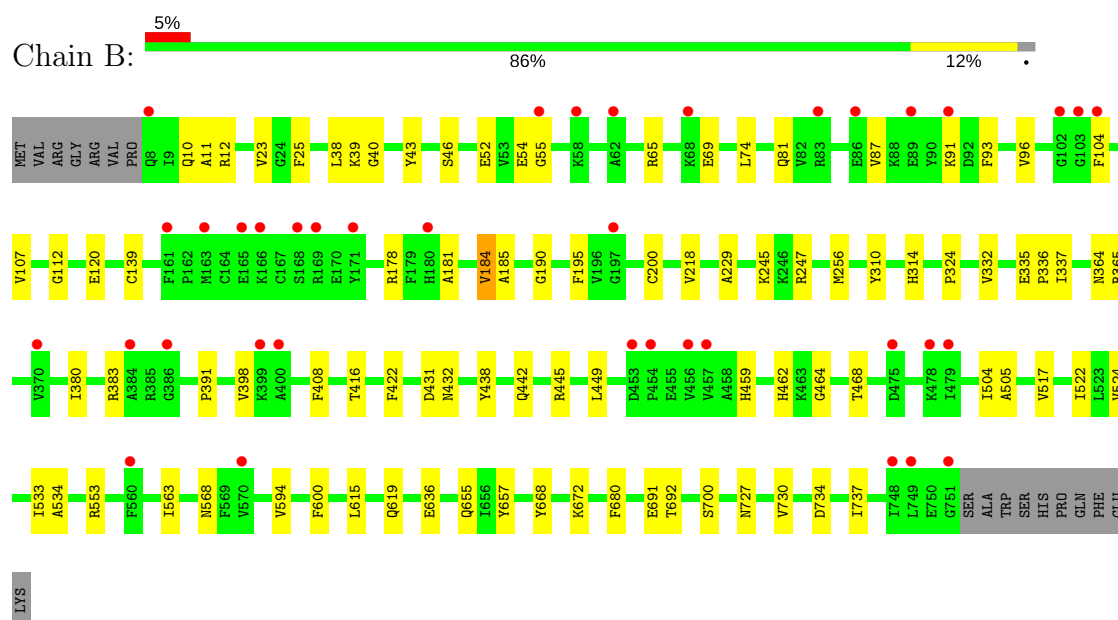
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

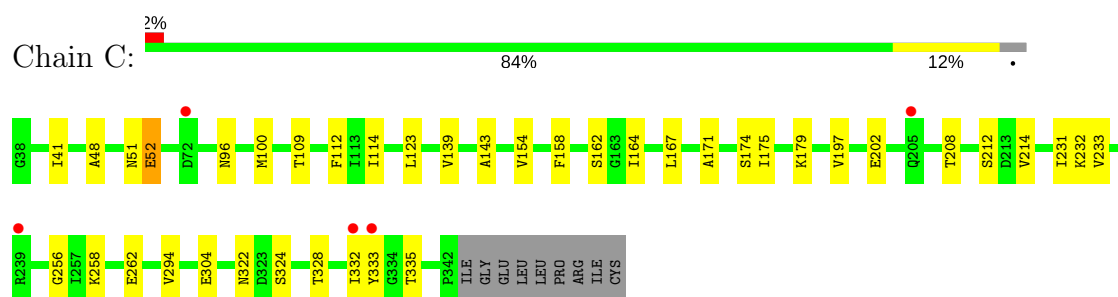
#### • Molecule 1: Hydrogenase maturation factor



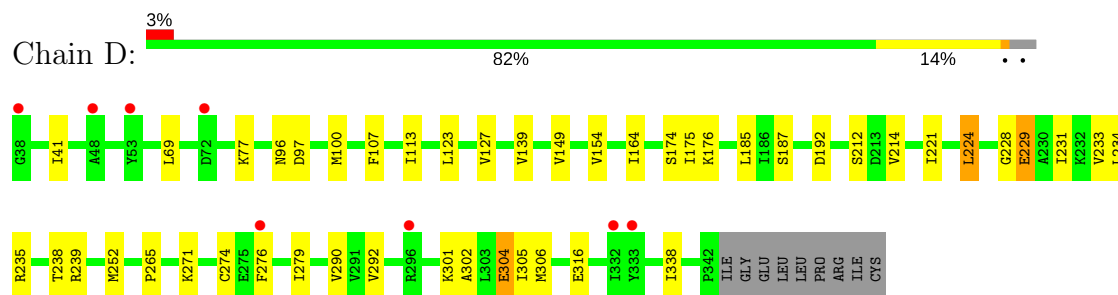
#### • Molecule 1: Hydrogenase maturation factor



#### • Molecule 2: Hydrogenase maturation factor



• Molecule 2: Hydrogenase maturation factor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.74Å 119.10Å 174.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.56 39.28 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.56) 97.9 (39.28-2.56)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.39 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.206 , 0.251 0.215 , 0.261	Depositor DCC
$R_{free}$ test set	3921 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, FE

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	0.48	0/6083	0.57	0/8193
1	B	0.42	0/6083	0.53	0/8193
2	C	0.44	0/2338	0.54	0/3155
2	D	0.42	0/2338	0.54	0/3155
All	All	0.44	0/16842	0.55	0/22696

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 [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	5964	0	5968	63	0
1	B	5964	0	5968	55	0
2	C	2305	0	2354	34	0
2	D	2305	0	2354	34	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	A	177	0	0	4	0
6	B	113	0	0	2	0
6	C	58	0	0	3	0
6	D	45	0	0	3	0
All	All	16939	0	16644	171	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 (171) 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:D:149:VAL:HG21	2:D:154:VAL:HG23	1.25	1.07
1:B:462:HIS:HD2	1:B:464:GLY:H	1.12	0.96
1:A:278:SER:O	1:A:281:ARG:HD3	1.74	0.87
2:D:149:VAL:CG2	2:D:154:VAL:HG23	2.06	0.85
1:B:615:LEU:H	1:B:619:GLN:NE2	1.75	0.83
2:D:149:VAL:HG21	2:D:154:VAL:CG2	2.08	0.81
1:A:331:ASN:HB2	1:A:335:GLU:OE2	1.85	0.75
1:B:615:LEU:H	1:B:619:GLN:HE22	1.33	0.75
1:B:553:ARG:NH2	2:D:276:PHE:O	2.21	0.73
1:B:398:VAL:HG21	1:B:416:THR:HB	1.73	0.70
1:B:462:HIS:CD2	1:B:464:GLY:H	2.04	0.70
1:A:462:HIS:HD2	1:A:464:GLY:H	1.39	0.69
1:B:364:ASN:HD21	1:B:445:ARG:HE	1.40	0.69
1:A:43:TYR:HB3	1:A:96:VAL:HG23	1.76	0.68
2:C:41:ILE:HG23	2:D:123:LEU:HD21	1.74	0.68
2:D:187:SER:HB3	2:D:290:VAL:H	1.60	0.66
2:D:304:GLU:OE1	2:D:305:ILE:HG23	1.96	0.65
1:B:365:ARG:HG2	1:B:438:TYR:CE2	2.32	0.65
2:C:256:GLY:HA3	2:C:324:SER:O	1.97	0.65
2:D:228:GLY:O	2:D:229:GLU:HB2	1.96	0.65
1:B:310:TYR:H	1:B:314:HIS:HD2	1.45	0.64
2:C:48:ALA:CB	2:D:127:VAL:HG12	2.28	0.64
1:A:185:ALA:HB1	1:A:190:GLY:HA3	1.80	0.64
1:A:247:ARG:HH21	2:C:332:ILE:HG13	1.62	0.64
2:C:158:PHE:HE2	2:D:154:VAL:HG22	1.63	0.63
2:D:107:PHE:HD2	2:D:164:ILE:HD11	1.64	0.62
1:A:240:THR:HG22	1:A:243:ARG:HH22	1.65	0.62
1:A:533:ILE:HG21	1:A:688:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:PHE:HE2	1:B:431:ASP:HB3	1.65	0.61
1:A:105:VAL:HG13	1:A:106:PRO:HD2	1.83	0.61
1:A:329:SER:HB2	1:A:337:ILE:CG2	2.31	0.60
1:A:553:ARG:HH22	1:A:584:GLN:HE22	1.49	0.60
2:D:274:CYS:HB3	2:D:279:ILE:O	2.02	0.60
1:A:10:GLN:HE21	1:A:12:ARG:HH22	1.50	0.59
1:B:23:VAL:HG12	1:B:74:LEU:HB2	1.85	0.59
1:A:553:ARG:NH2	1:A:584:GLN:HE22	2.01	0.58
1:B:636:GLU:H	1:B:655:GLN:HE22	1.49	0.58
1:B:43:TYR:HB3	1:B:96:VAL:HG23	1.87	0.57
2:C:258:LYS:HE2	2:C:328:THR:OG1	2.04	0.57
1:B:408:PHE:CE2	1:B:431:ASP:HB3	2.39	0.57
2:C:322:ASN:ND2	6:C:542:HOH:O	2.37	0.57
1:B:245:LYS:HD2	1:B:332:VAL:O	2.05	0.56
2:D:301:LYS:O	2:D:304:GLU:HG3	2.03	0.56
1:A:408:PHE:HE2	1:A:431:ASP:HB3	1.69	0.56
1:A:278:SER:O	1:A:281:ARG:CD	2.50	0.56
1:B:380:ILE:HD13	1:B:383:ARG:HG3	1.89	0.55
2:D:212:SER:OG	2:D:214:VAL:HG23	2.07	0.55
1:A:524:VAL:HG23	1:A:533:ILE:HG13	1.87	0.54
1:B:256:MET:HG2	1:B:324:PRO:HB3	1.89	0.54
1:A:247:ARG:HH21	2:C:332:ILE:CG1	2.21	0.54
2:C:48:ALA:HB3	2:D:127:VAL:CG1	2.38	0.54
1:B:39:LYS:HG2	1:B:54:GLU:O	2.08	0.53
1:B:517:VAL:HB	1:B:594:VAL:HG12	1.90	0.53
1:A:197:GLY:HA3	1:A:354:VAL:HG12	1.90	0.53
1:A:208:VAL:HG13	1:A:218:VAL:HG11	1.90	0.53
1:B:112:GLY:O	1:B:139:CYS:HB2	2.08	0.53
2:D:221:ILE:HD12	2:D:234:LEU:HD13	1.90	0.53
1:A:456:VAL:HG12	1:A:477:PRO:HG2	1.91	0.53
1:B:459:HIS:CD2	1:B:468:THR:HG23	2.44	0.53
1:B:727:ASN:HB3	1:B:730:VAL:O	2.09	0.52
2:C:256:GLY:CA	2:C:324:SER:O	2.58	0.52
1:A:36:TYR:HB3	1:A:59:ASP:HB3	1.92	0.52
1:A:399:LYS:HD2	1:A:750:GLU:HA	1.92	0.51
2:C:164:ILE:HD12	2:D:69:LEU:HD22	1.92	0.51
1:A:364:ASN:OD1	1:A:445:ARG:HD2	2.10	0.51
2:D:113:ILE:HG22	2:D:154:VAL:HG21	1.92	0.51
1:B:107:VAL:HG21	1:B:449:LEU:HG	1.93	0.50
1:A:589:ILE:HD11	2:C:202:GLU:HG3	1.93	0.50
2:C:174:SER:O	2:C:233:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:O	1:B:91:LYS:HD3	2.12	0.49
2:D:224:LEU:O	2:D:231:ILE:HD11	2.12	0.49
2:C:114:ILE:HD13	2:D:41:ILE:HG21	1.95	0.49
1:B:245:LYS:CE	6:B:902:HOH:O	2.61	0.48
2:C:48:ALA:CB	2:D:127:VAL:CG1	2.90	0.48
2:C:109:THR:HG22	2:C:143:ALA:HB3	1.95	0.48
1:B:10:GLN:OE1	1:B:12:ARG:NH1	2.46	0.48
1:B:40:GLY:O	1:B:93:PHE:HA	2.13	0.48
1:B:691:GLU:HG3	1:B:692:THR:HG23	1.95	0.48
2:C:96:ASN:O	2:C:100:MET:HG2	2.14	0.48
1:A:332:VAL:O	1:A:335:GLU:OE1	2.31	0.48
2:C:154:VAL:HG23	2:C:158:PHE:CE2	2.49	0.48
1:A:247:ARG:HD2	2:C:335:THR:OG1	2.14	0.48
1:A:337:ILE:O	1:A:365:ARG:HD3	2.13	0.48
1:B:245:LYS:HE2	6:B:902:HOH:O	2.15	0.47
1:A:149:ILE:HB	1:A:150:PRO:HA	1.97	0.47
1:B:364:ASN:HD21	1:B:445:ARG:NE	2.10	0.47
1:A:468:THR:HG22	1:A:472:LYS:HE2	1.97	0.47
1:B:522:ILE:HB	1:B:534:ALA:HB3	1.97	0.47
1:A:181:ALA:HB3	1:A:184:VAL:HG13	1.97	0.47
2:C:231:ILE:HD13	2:C:294:VAL:HG12	1.97	0.47
1:A:432:ASN:ND2	1:A:435:ALA:H	2.13	0.47
2:C:232:LYS:NZ	6:C:533:HOH:O	2.47	0.47
1:A:32:ILE:HD12	6:A:1021:HOH:O	2.15	0.47
1:B:364:ASN:HD22	1:B:442:GLN:HE22	1.62	0.47
1:B:459:HIS:HD2	1:B:468:THR:HG23	1.79	0.46
1:B:11:ALA:HB2	1:B:54:GLU:HG2	1.97	0.46
2:D:185:LEU:HB2	2:D:292:VAL:HG22	1.97	0.46
1:B:310:TYR:H	1:B:314:HIS:CD2	2.29	0.46
1:B:668:TYR:CZ	1:B:672:LYS:HD2	2.50	0.46
2:D:175:ILE:HD13	2:D:235:ARG:CZ	2.46	0.46
1:A:534:ALA:HA	1:A:645:TYR:O	2.16	0.46
1:A:534:ALA:HB2	1:A:645:TYR:HB2	1.98	0.46
1:B:734:ASP:HA	1:B:737:ILE:HG12	1.98	0.46
1:A:40:GLY:O	1:A:93:PHE:HA	2.16	0.46
1:A:26:ARG:HB2	1:A:27:PRO:HD3	1.98	0.45
1:A:289:LYS:O	1:A:292:LYS:HE2	2.17	0.45
1:B:120:GLU:OE2	1:B:178:ARG:NH2	2.50	0.45
1:A:608:ILE:HG13	1:A:610:VAL:HG23	1.97	0.45
2:C:109:THR:OG1	2:C:162:SER:HB2	2.17	0.45
2:D:174:SER:O	2:D:233:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:256:GLY:N	2:C:324:SER:O	2.50	0.45
1:B:337:ILE:O	1:B:365:ARG:HD3	2.17	0.45
2:C:212:SER:OG	2:C:214:VAL:HG23	2.17	0.45
2:C:332:ILE:O	2:C:333:TYR:HB2	2.16	0.45
1:A:14:ILE:HB	1:A:51:ILE:HB	1.99	0.45
2:D:77:LYS:HE3	6:D:516:HOH:O	2.17	0.44
1:A:105:VAL:CG1	1:A:106:PRO:HD2	2.48	0.44
1:A:620:ALA:O	1:A:624:LEU:HB2	2.16	0.44
2:C:167:LEU:HG	2:C:171:ALA:HB3	2.00	0.44
1:B:335:GLU:HB2	1:B:336:PRO:HD2	1.99	0.44
1:A:329:SER:HB2	1:A:337:ILE:HG21	1.99	0.44
1:B:40:GLY:HA3	1:B:52:GLU:O	2.18	0.44
2:C:262:GLU:H	2:C:262:GLU:CD	2.21	0.44
1:B:181:ALA:HB3	1:B:184:VAL:HG13	2.00	0.43
1:A:104:PHE:HB3	1:A:105:VAL:HA	1.99	0.43
1:B:505:ALA:HA	1:B:700:SER:O	2.18	0.43
1:A:522:ILE:HG21	1:A:688:ILE:HD13	2.00	0.43
1:A:625:GLU:O	1:A:628:MET:HG2	2.18	0.43
2:C:154:VAL:CG2	2:C:158:PHE:CE2	3.01	0.43
2:D:265:PRO:HG3	2:D:316:GLU:HB2	2.00	0.43
1:B:195:PHE:CD2	1:B:200:CYS:HB2	2.53	0.43
1:A:38:LEU:HD23	1:A:55:GLY:HA3	2.01	0.43
1:B:185:ALA:HB1	1:B:190:GLY:HA3	2.01	0.43
1:B:218:VAL:HG22	1:B:229:ALA:HB3	2.00	0.43
2:D:302:ALA:O	2:D:306:MET:HG3	2.19	0.42
1:A:203:ASP:OD1	1:A:206:LYS:HD3	2.20	0.42
1:A:248:TYR:HB3	6:A:909:HOH:O	2.18	0.42
2:C:179:LYS:HE2	6:C:533:HOH:O	2.20	0.42
1:B:38:LEU:HD23	1:B:55:GLY:HA3	2.01	0.42
1:A:364:ASN:OD1	1:A:445:ARG:CD	2.67	0.42
1:A:210:LYS:HD3	6:A:1062:HOH:O	2.19	0.42
1:B:568:ASN:HB3	1:B:657:TYR:OH	2.19	0.42
2:C:123:LEU:HD21	2:D:41:ILE:HG23	2.00	0.42
1:A:277:LEU:O	1:A:281:ARG:NH1	2.53	0.42
2:C:52:GLU:H	2:C:52:GLU:CD	2.22	0.42
1:A:408:PHE:CE2	1:A:431:ASP:HB3	2.52	0.42
2:D:229:GLU:HB3	6:D:541:HOH:O	2.19	0.42
1:A:396:LYS:HB2	1:A:396:LYS:HE3	1.86	0.42
1:A:398:VAL:HG21	1:A:416:THR:HB	2.02	0.42
1:A:149:ILE:HD11	1:A:451:ARG:HD3	2.01	0.42
2:D:96:ASN:O	2:D:100:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:ASN:HB2	2:C:52:GLU:OE1	2.20	0.41
1:A:727:ASN:HB3	1:A:730:VAL:O	2.20	0.41
1:B:65:ARG:O	1:B:69:GLU:HG2	2.21	0.41
1:B:524:VAL:HG23	1:B:533:ILE:HG13	2.02	0.41
2:C:158:PHE:CE2	2:D:154:VAL:HG22	2.49	0.41
2:D:176:LYS:HG2	2:D:252:MET:O	2.21	0.41
1:A:252:PHE:HB3	1:A:326:VAL:HG13	2.01	0.41
1:A:63:PHE:HA	6:A:1021:HOH:O	2.21	0.41
1:B:504:ILE:HG12	1:B:522:ILE:HG12	2.02	0.41
2:C:112:PHE:HB3	2:C:114:ILE:HD11	2.03	0.41
1:A:154:ALA:O	1:A:159:LYS:HD3	2.20	0.41
1:A:402:ILE:HG12	1:A:456:VAL:CG2	2.51	0.41
1:B:432:ASN:HA	2:D:338:ILE:HG23	2.03	0.41
1:B:247:ARG:NH1	6:D:536:HOH:O	2.53	0.41
1:B:391:PRO:HB3	1:B:422:PHE:CD1	2.56	0.41
1:B:43:TYR:HB3	1:B:96:VAL:CG2	2.51	0.41
1:A:123:ASP:HA	1:A:124:PRO:HD3	1.94	0.41
1:A:281:ARG:HD2	1:A:281:ARG:HA	1.89	0.40
1:A:700:SER:OG	1:A:727:ASN:ND2	2.54	0.40
2:D:238:THR:O	2:D:239:ARG:C	2.58	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	742/761 (98%)	701 (94%)	41 (6%)	0	100	100
1	B	742/761 (98%)	702 (95%)	38 (5%)	2 (0%)	44	66
2	C	303/314 (96%)	283 (93%)	20 (7%)	0	100	100
2	D	303/314 (96%)	291 (96%)	11 (4%)	1 (0%)	44	66
All	All	2090/2150 (97%)	1977 (95%)	110 (5%)	3 (0%)	55	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	SER
1	B	104	PHE
2	D	229	GLU

### 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	646/661 (98%)	629 (97%)	17 (3%)	51	75
1	B	646/661 (98%)	639 (99%)	7 (1%)	78	90
2	C	248/256 (97%)	242 (98%)	6 (2%)	54	77
2	D	248/256 (97%)	242 (98%)	6 (2%)	54	77
All	All	1788/1834 (98%)	1752 (98%)	36 (2%)	60	81

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	A	35	LYS
1	A	70	ASN
1	A	166	LYS
1	A	184	VAL
1	A	202	ASP
1	A	203	ASP
1	A	235	ASP
1	A	281	ARG
1	A	332	VAL
1	A	351	ILE
1	A	461	MET
1	A	477	PRO
1	A	600	PHE
1	A	611	ARG
1	A	680	PHE
1	A	712	ARG

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Mol	Chain	Res	Type
1	B	25	PHE
1	B	81	GLN
1	B	87	VAL
1	B	184	VAL
1	B	563	ILE
1	B	600	PHE
1	B	680	PHE
2	C	52	GLU
2	C	139	VAL
2	C	175	ILE
2	C	197	VAL
2	C	208	THR
2	C	304	GLU
2	D	97	ASP
2	D	139	VAL
2	D	192	ASP
2	D	224	LEU
2	D	271	LYS
2	D	304	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	135	ASN
1	A	411	ASN
1	A	432	ASN
1	A	437	ASN
1	A	462	HIS
1	A	496	ASN
1	A	562	ASN
1	A	568	ASN
1	A	584	GLN
1	A	705	GLN
1	A	727	ASN
1	B	135	ASN
1	B	175	HIS
1	B	314	HIS
1	B	364	ASN
1	B	411	ASN
1	B	432	ASN
1	B	459	HIS

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Mol	Chain	Res	Type
1	B	462	HIS
1	B	495	HIS
1	B	562	ASN
1	B	584	GLN
1	B	619	GLN
1	B	655	GLN
1	B	727	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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	744/761 (97%)	0.09	22 (2%)	51	48	28, 50, 80, 114	2 (0%)
1	B	744/761 (97%)	0.34	38 (5%)	29	25	40, 62, 89, 105	2 (0%)
2	C	305/314 (97%)	0.08	5 (1%)	72	71	36, 53, 78, 104	5 (1%)
2	D	305/314 (97%)	0.21	8 (2%)	56	54	40, 63, 91, 110	5 (1%)
All	All	2098/2150 (97%)	0.19	73 (3%)	44	41	28, 57, 87, 114	14 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	333	TYR	7.7
1	B	457	VAL	6.4
2	D	333	TYR	5.6
1	A	8	GLN	5.2
1	A	9	ILE	4.7
1	A	201	PHE	4.6
1	B	197	GLY	4.5
1	B	456	VAL	4.4
1	B	165	GLU	4.2
1	B	91	LYS	4.0
1	B	8	GLN	3.9
1	B	748	ILE	3.9
1	B	103	GLY	3.7
2	C	72	ASP	3.7
1	B	751	GLY	3.6
1	A	475	ASP	3.5
1	A	37	ASN	3.5
1	A	60	ILE	3.5
1	A	175	HIS	3.4
2	D	72	ASP	3.2
1	B	478	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	560	PHE	3.1
2	D	48	ALA	3.1
1	B	55	GLY	3.1
1	B	453	ASP	3.1
2	D	53	TYR	3.1
1	B	169	ARG	3.0
1	A	104	PHE	3.0
1	B	749	LEU	3.0
1	B	370	VAL	2.9
1	B	454	PRO	2.9
1	A	33	ALA	2.9
2	C	239	ARG	2.8
1	B	171	TYR	2.7
2	D	332	ILE	2.7
1	B	163	MET	2.7
1	B	161	PHE	2.7
1	A	61	GLU	2.7
1	B	104	PHE	2.7
1	B	86	GLU	2.6
1	B	68	LYS	2.6
1	B	384	ALA	2.5
1	A	84	GLU	2.5
2	C	332	ILE	2.5
2	D	296	ARG	2.5
1	A	340	ASP	2.5
1	B	180	HIS	2.5
1	B	570	VAL	2.4
2	D	276	PHE	2.4
1	B	399	LYS	2.3
1	A	56	GLU	2.3
1	A	91	LYS	2.3
1	B	89	GLU	2.3
2	D	38	GLY	2.3
1	B	62	ALA	2.3
1	B	386	GLY	2.2
2	C	205	GLN	2.2
1	A	57	GLU	2.2
1	A	36	TYR	2.2
1	B	58	LYS	2.2
1	B	102	GLY	2.2
1	B	400	ALA	2.1
1	B	475	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	65	ARG	2.1
1	B	166	LYS	2.1
1	B	83	ARG	2.1
1	A	34	GLN	2.1
1	B	479	ILE	2.1
1	A	86	GLU	2.1
1	A	38	LEU	2.1
1	B	168	SER	2.0
1	A	35	LYS	2.0
1	A	106	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	D	401	1/1	0.75	0.27	4.40	34,34,34,34	0
3	ZN	A	801	1/1	1.00	0.11	-1.01	42,42,42,42	0
4	FE	B	803	1/1	0.89	0.12	-1.04	61,61,61,61	0
3	ZN	A	802	1/1	0.99	0.09	-1.21	56,56,56,56	0
4	FE	A	803	1/1	0.97	0.14	-2.02	43,43,43,43	0
3	ZN	B	801	1/1	0.98	0.09	-2.36	64,64,64,64	0
3	ZN	B	802	1/1	0.99	0.04	-2.71	89,89,89,89	0
5	MG	C	401	1/1	0.94	0.32	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.