



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:49 AM GMT

PDB ID : 2IBG
Title : Crystal Structure of Hedgehog Bound to the FNIII Domains of Ihog
Authors : McLellan, J.S.; Leahy, D.J.
Deposited on : 2006-09-11
Resolution : 2.20 Å(reported)

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

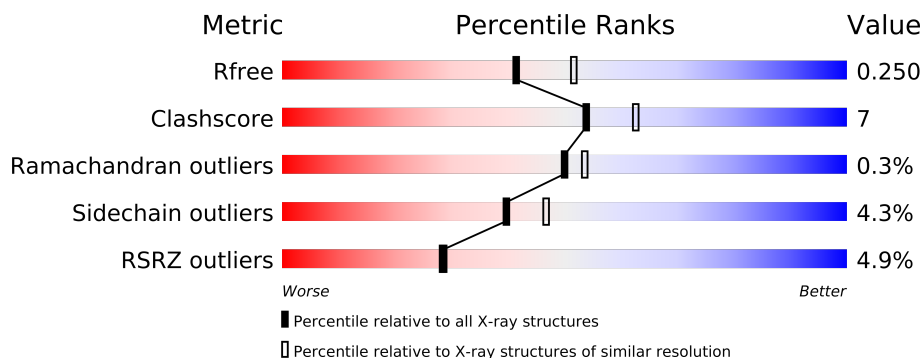
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. 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	214	
1	B	214	
1	C	214	
1	D	214	
2	E	150	
2	F	150	
2	G	150	
2	H	150	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11644 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 CG9211-PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1715	1095	290	325	5			
1	B	213	Total	C	N	O	S	0	0	0
			1705	1089	288	323	5			
1	C	213	Total	C	N	O	S	0	0	0
			1705	1089	288	323	5			
1	D	213	Total	C	N	O	S	0	0	0
			1705	1089	288	323	5			

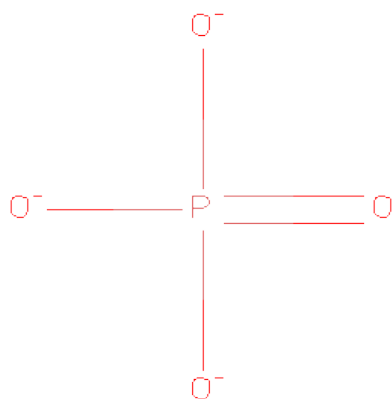
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	SER	-	CLONING ARTIFACT	UNP Q9VM64
A	465	THR	-	CLONING ARTIFACT	UNP Q9VM64
B	464	SER	-	CLONING ARTIFACT	UNP Q9VM64
B	465	THR	-	CLONING ARTIFACT	UNP Q9VM64
C	464	SER	-	CLONING ARTIFACT	UNP Q9VM64
C	465	THR	-	CLONING ARTIFACT	UNP Q9VM64
D	464	SER	-	CLONING ARTIFACT	UNP Q9VM64
D	465	THR	-	CLONING ARTIFACT	UNP Q9VM64

- Molecule 2 is a protein called Protein hedgehog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	142	Total	C	N	O	S	0	0	0
			1161	732	206	218	5			
2	F	132	Total	C	N	O	S	0	0	0
			1070	679	190	196	5			
2	G	134	Total	C	N	O	S	0	0	0
			1092	694	191	202	5			
2	H	140	Total	C	N	O	S	0	0	0
			1142	722	201	214	5			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

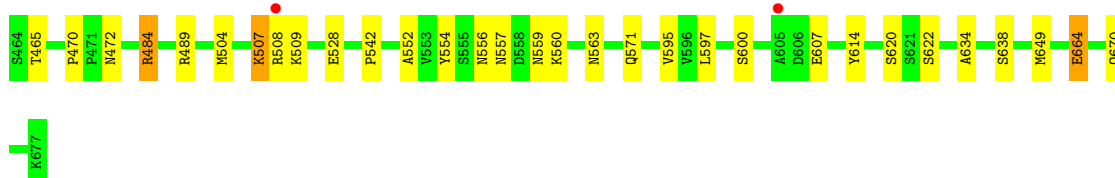
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total 66	O 66	0	0
4	B	48	Total 48	O 48	0	0
4	C	63	Total 63	O 63	0	0
4	D	54	Total 54	O 54	0	0
4	E	28	Total 28	O 28	0	0
4	F	8	Total 8	O 8	0	0
4	G	12	Total 12	O 12	0	0
4	H	10	Total 10	O 10	0	0

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: CG9211-PA

Chain A: 



- Molecule 1: CG9211-PA

Chain B: 



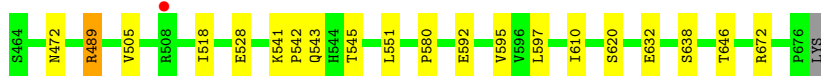
- Molecule 1: CG9211-PA

Chain C: 



- Molecule 1: CG9211-PA

Chain D: 



- Molecule 2: Protein hedgehog

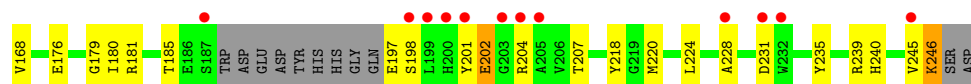
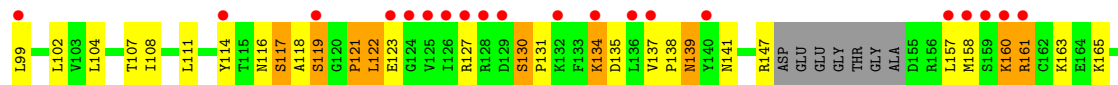
Chain E: 





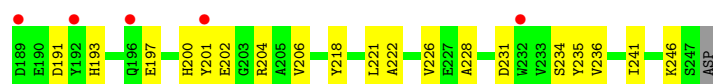
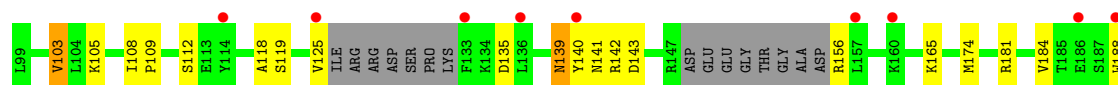
• Molecule 2: Protein hedgehog

Chain F:



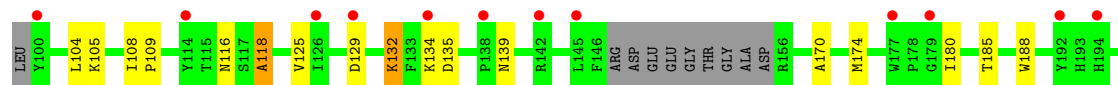
• Molecule 2: Protein hedgehog

Chain G:



• Molecule 2: Protein hedgehog

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.35Å 70.00Å 155.69Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	37.68 – 2.20 37.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (37.68-2.20) 92.2 (37.68-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.246 0.202 , 0.250	Depositor DCC
R_{free} test set	3864 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.4	EDS
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 82870 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11644	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: PO4

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	0.68	0/1764	0.73	0/2397
1	B	0.64	0/1754	0.68	0/2386
1	C	0.60	0/1754	0.67	0/2386
1	D	0.64	0/1754	0.71	0/2386
2	E	0.51	0/1187	0.66	1/1603 (0.1%)
2	F	1.98	31/1090 (2.8%)	1.07	7/1470 (0.5%)
2	G	0.52	0/1116	0.60	0/1508
2	H	0.48	0/1168	0.61	0/1578
All	All	0.83	31/11587 (0.3%)	0.72	8/15714 (0.1%)

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
2	F	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	117	SER	CB-OG	23.21	1.72	1.42
2	F	202	GLU	CD-OE2	20.15	1.47	1.25
2	F	161	ARG	CZ-NH1	18.89	1.57	1.33
2	F	123	GLU	CD-OE1	17.42	1.44	1.25
2	F	121	PRO	C-N	15.07	1.68	1.34
2	F	197	GLU	CD-OE1	10.91	1.37	1.25
2	F	197	GLU	CG-CD	10.39	1.67	1.51
2	F	161	ARG	NE-CZ	9.84	1.45	1.33
2	F	114	TYR	CG-CD2	9.60	1.51	1.39
2	F	197	GLU	CD-OE2	9.58	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	197	GLU	C-O	9.56	1.41	1.23
2	F	114	TYR	CE1-CZ	9.26	1.50	1.38
2	F	246	LYS	C-O	9.23	1.40	1.23
2	F	114	TYR	CE2-CZ	9.04	1.50	1.38
2	F	119	SER	CB-OG	8.99	1.53	1.42
2	F	117	SER	C-N	8.62	1.53	1.34
2	F	135	ASP	CG-OD1	8.37	1.44	1.25
2	F	114	TYR	CG-CD1	8.29	1.50	1.39
2	F	123	GLU	CD-OE2	7.29	1.33	1.25
2	F	130	SER	CA-CB	6.95	1.63	1.52
2	F	122	LEU	C-O	6.37	1.35	1.23
2	F	116	ASN	C-O	6.34	1.35	1.23
2	F	161	ARG	CG-CD	6.09	1.67	1.51
2	F	165	LYS	CD-CE	6.08	1.66	1.51
2	F	161	ARG	CZ-NH2	6.08	1.41	1.33
2	F	117	SER	C-O	5.57	1.33	1.23
2	F	134	LYS	CD-CE	5.42	1.64	1.51
2	F	130	SER	C-O	5.39	1.33	1.23
2	F	201	TYR	CG-CD1	5.36	1.46	1.39
2	F	131	PRO	N-CD	5.28	1.55	1.47
2	F	201	TYR	CE2-CZ	5.08	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	161	ARG	NE-CZ-NH2	-19.50	110.55	120.30
2	F	121	PRO	O-C-N	8.21	135.84	122.70
2	F	121	PRO	CA-C-N	-6.54	102.82	117.20
2	F	161	ARG	NE-CZ-NH1	5.83	123.21	120.30
2	F	161	ARG	NH1-CZ-NH2	5.30	125.23	119.40
2	F	122	LEU	CA-CB-CG	5.24	127.36	115.30
2	E	102	LEU	CA-CB-CG	5.19	127.23	115.30
2	F	202	GLU	OE1-CD-OE2	-5.10	117.18	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	202	GLU	Sidechain

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	1715	0	1674	25	0
1	B	1705	0	1661	21	0
1	C	1705	0	1661	15	0
1	D	1705	0	1661	18	0
2	E	1161	0	1137	16	0
2	F	1070	0	1080	29	0
2	G	1092	0	1073	22	0
2	H	1142	0	1120	18	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	15	0	0	0	0
3	F	5	0	0	1	0
3	H	5	0	0	0	0
4	A	66	0	0	2	0
4	B	48	0	0	0	0
4	C	63	0	0	1	0
4	D	54	0	0	1	0
4	E	28	0	0	0	0
4	F	8	0	0	0	0
4	G	12	0	0	0	0
4	H	10	0	0	0	0
All	All	11644	0	11067	154	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 7.

All (154) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:121:PRO:C	2:F:122:LEU:N	1.68	1.46
2:F:117:SER:OG	2:F:117:SER:CB	1.72	1.34
2:H:185:THR:OG1	2:H:207:THR:HG22	1.68	0.93
1:C:580:PRO:HG2	1:C:610:ILE:HD11	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:168:VAL:HG23	2:F:228:ALA:HB1	1.67	0.76
1:D:542:PRO:HB3	4:D:274:HOH:O	1.87	0.72
2:G:125:VAL:HG13	2:G:201:TYR:HB3	1.72	0.72
1:A:620:SER:HB3	1:A:670:GLN:NE2	2.05	0.72
2:E:147:ARG:HG2	2:E:185:THR:HA	1.72	0.70
2:F:121:PRO:CA	2:F:122:LEU:N	2.55	0.69
2:G:221:LEU:HD23	2:G:241:ILE:HD12	1.76	0.68
1:B:607:GLU:HG2	1:B:634:ALA:HB1	1.76	0.66
2:F:139:ASN:HD22	2:F:141:ASN:H	1.45	0.64
1:A:484:ARG:NH2	1:D:528:GLU:HB3	2.11	0.64
1:B:505:VAL:HG21	1:B:567:LYS:HG2	1.79	0.62
2:H:125:VAL:HG13	2:H:201:TYR:HB3	1.80	0.62
2:G:118:ALA:O	2:G:231:ASP:HB3	2.00	0.62
1:A:620:SER:HB3	1:A:670:GLN:HE22	1.63	0.61
1:A:489:ARG:CB	1:D:472:ASN:OD1	2.48	0.61
1:B:501:GLN:HE22	1:B:549:ARG:HH21	1.49	0.61
1:D:551:LEU:HD22	2:G:103:VAL:HG13	1.82	0.61
2:F:160:LYS:HA	2:F:160:LYS:HE3	1.83	0.60
2:G:234:SER:OG	2:G:236:VAL:HG22	2.02	0.60
2:E:125:VAL:HG13	2:E:201:TYR:HB3	1.84	0.60
1:D:489:ARG:NH1	1:D:528:GLU:O	2.35	0.59
2:E:139:ASN:ND2	2:E:141:ASN:H	2.01	0.59
2:F:185:THR:OG1	2:F:207:THR:HG22	2.03	0.59
1:C:607:GLU:HG2	1:C:634:ALA:HB1	1.84	0.58
1:A:620:SER:CB	1:A:670:GLN:NE2	2.65	0.58
2:E:139:ASN:HD21	2:E:141:ASN:HB2	1.68	0.58
2:F:119:SER:O	2:F:246:LYS:HA	2.03	0.58
2:E:122:LEU:HD23	2:E:199:LEU:HD23	1.86	0.58
2:F:121:PRO:C	2:F:122:LEU:CA	2.70	0.57
2:E:116:ASN:OD1	2:E:116:ASN:N	2.37	0.57
2:F:179:GLY:HA2	3:F:410:PO4:P	2.44	0.56
1:B:486:MET:SD	1:C:486:MET:SD	3.04	0.56
1:A:489:ARG:HB2	1:D:472:ASN:OD1	2.06	0.55
2:H:104:LEU:O	2:H:105:LYS:HB2	2.06	0.55
1:A:528:GLU:HG2	1:D:632:GLU:HG2	1.87	0.55
2:H:206:VAL:HG22	2:H:208:ILE:HG23	1.89	0.55
2:E:139:ASN:HD21	2:E:141:ASN:CB	2.19	0.55
1:C:516:ASP:O	4:C:239:HOH:O	2.19	0.54
2:E:104:LEU:HG	2:E:105:LYS:HG2	1.88	0.54
1:B:501:GLN:HE21	1:B:549:ARG:HE	1.55	0.54
1:A:489:ARG:HB3	1:D:472:ASN:OD1	2.07	0.54
1:C:587:ILE:HD13	1:C:652:PHE:CD1	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:507:LYS:O	1:A:509:LYS:HG2	2.09	0.52
1:C:556:ASN:O	1:C:557:ASN:HB2	2.09	0.52
2:F:137:VAL:HG21	2:F:160:LYS:HZ1	1.75	0.52
1:A:664:GLU:HG3	4:A:79:HOH:O	2.10	0.52
2:G:191:ASP:HB3	2:G:193:HIS:CD2	2.45	0.52
1:A:607:GLU:HG2	1:A:634:ALA:HB1	1.93	0.51
2:E:139:ASN:HD22	2:E:139:ASN:C	2.15	0.51
2:F:204:ARG:HG2	2:F:245:VAL:HG23	1.91	0.51
1:B:522:LYS:HB3	1:B:523:PRO:HA	1.93	0.50
1:A:556:ASN:O	1:A:557:ASN:HB2	2.11	0.50
1:A:472:ASN:OD1	1:D:489:ARG:HB3	2.10	0.50
1:A:542:PRO:HB3	4:A:25:HOH:O	2.11	0.50
1:B:501:GLN:NE2	1:B:549:ARG:HE	2.09	0.50
1:D:580:PRO:HG2	1:D:610:ILE:HD11	1.93	0.50
1:B:470:PRO:HG3	1:B:563:ASN:HB2	1.94	0.50
1:B:503:ARG:HD3	1:B:509:LYS:HG3	1.94	0.50
1:D:489:ARG:NH1	1:D:528:GLU:C	2.66	0.49
2:E:143:ASP:HB3	2:E:174:MET:CE	2.43	0.49
1:B:503:ARG:CD	1:B:509:LYS:HG3	2.43	0.49
1:A:470:PRO:HG3	1:A:563:ASN:HB2	1.95	0.49
2:H:231:ASP:CG	2:H:246:LYS:HG3	2.32	0.48
2:G:119:SER:O	2:G:246:LYS:HA	2.13	0.48
1:B:597:LEU:O	1:B:638:SER:HA	2.13	0.48
2:H:118:ALA:O	2:H:231:ASP:HB3	2.14	0.48
2:F:158:MET:CE	2:F:163:LYS:HA	2.43	0.48
2:H:207:THR:HG23	2:H:240:HIS:CG	2.48	0.47
2:G:231:ASP:CG	2:G:246:LYS:HG3	2.34	0.47
1:B:508:ARG:O	1:B:510:ASN:N	2.48	0.47
1:B:524:LYS:HE3	1:B:525:TRP:CZ2	2.50	0.47
2:F:127:ARG:H	2:F:130:SER:HB2	1.80	0.47
1:C:580:PRO:CG	1:C:610:ILE:HD11	2.40	0.47
1:D:489:ARG:NH1	1:D:528:GLU:HA	2.30	0.47
1:D:592:GLU:O	1:D:646:THR:HA	2.15	0.47
1:C:672:ARG:HD2	1:C:673:THR:O	2.15	0.46
2:G:108:ILE:HA	2:G:109:PRO:C	2.35	0.46
2:H:170:ALA:O	2:H:174:MET:HG3	2.14	0.46
2:F:102:LEU:HD11	2:F:108:ILE:HD12	1.97	0.46
2:F:139:ASN:ND2	2:F:141:ASN:H	2.11	0.46
2:H:208:ILE:HG13	2:H:241:ILE:HB	1.98	0.46
2:F:220:MET:HE3	2:F:220:MET:O	2.15	0.46
1:A:620:SER:OG	1:A:670:GLN:NE2	2.49	0.46
2:G:191:ASP:HB3	2:G:193:HIS:HD2	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:595:VAL:HG21	1:B:652:PHE:CZ	2.51	0.45
1:C:559:ASN:HD21	2:H:104:LEU:H	1.63	0.45
2:G:139:ASN:ND2	2:G:141:ASN:H	2.14	0.45
2:H:188:TRP:HA	2:H:200:HIS:O	2.17	0.45
2:G:202:GLU:HB2	2:G:204:ARG:HG3	1.98	0.45
2:F:207:THR:HG23	2:F:240:HIS:CD2	2.52	0.45
2:G:105:LYS:HA	2:G:105:LYS:HD3	1.82	0.45
2:G:143:ASP:CG	2:G:174:MET:HE1	2.37	0.45
1:B:556:ASN:O	1:B:557:ASN:HB2	2.16	0.45
1:C:646:THR:HG21	1:C:676:PRO:HG3	1.98	0.45
2:F:176:GLU:HG3	2:F:224:LEU:HD11	1.99	0.45
2:E:171:TYR:HA	2:E:174:MET:HE3	1.99	0.45
1:B:620:SER:OG	1:B:670:GLN:NE2	2.50	0.45
1:C:597:LEU:O	1:C:638:SER:HA	2.16	0.44
1:D:542:PRO:O	1:D:543:GLN:HB2	2.16	0.44
1:B:664:GLU:OE2	1:B:664:GLU:HA	2.18	0.44
1:A:504:MET:HB2	1:A:509:LYS:HG3	2.00	0.44
1:B:538:THR:O	1:B:539:ASP:HB2	2.17	0.44
2:E:139:ASN:HD22	2:E:141:ASN:H	1.65	0.44
2:F:218:TYR:HE2	2:F:239:ARG:O	2.00	0.44
1:A:620:SER:OG	1:A:649:MET:HG3	2.17	0.44
2:G:142:ARG:O	2:G:142:ARG:HG2	2.17	0.44
2:E:143:ASP:O	2:E:181:ARG:HD2	2.17	0.44
1:B:526:ASN:OD1	1:B:531:LYS:HA	2.18	0.44
2:F:158:MET:HE1	2:F:163:LYS:HA	2.00	0.43
2:F:147:ARG:HB3	2:F:185:THR:HA	2.00	0.43
2:G:165:LYS:HG3	2:G:228:ALA:O	2.18	0.43
1:C:507:LYS:H	1:C:507:LYS:HG2	1.70	0.43
2:H:207:THR:HG23	2:H:240:HIS:HB2	2.00	0.43
2:H:108:ILE:HA	2:H:109:PRO:C	2.38	0.43
2:F:180:ILE:HD12	2:F:180:ILE:N	2.33	0.43
1:C:569:TYR:CE2	1:C:571:GLN:NE2	2.86	0.43
1:B:523:PRO:HD3	1:B:643:PRO:HD2	1.99	0.43
2:F:118:ALA:O	2:F:231:ASP:HB3	2.18	0.43
2:H:215:GLN:NE2	2:H:238:ARG:O	2.52	0.43
2:G:184:VAL:HG13	2:G:206:VAL:HG23	1.99	0.43
1:C:542:PRO:C	1:C:543:GLN:HG2	2.39	0.42
1:D:541:LYS:HA	1:D:542:PRO:HD3	1.87	0.42
2:E:180:ILE:HD12	2:E:210:THR:HB	2.02	0.42
2:G:234:SER:OG	2:G:236:VAL:CG2	2.67	0.42
2:F:161:ARG:HH21	2:F:231:ASP:CG	2.23	0.42
2:H:206:VAL:CG2	2:H:208:ILE:HG23	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:505:VAL:HG22	1:D:545:THR:HB	2.02	0.42
1:A:597:LEU:O	1:A:638:SER:HA	2.19	0.42
2:H:213:ARG:HA	2:H:218:TYR:OH	2.20	0.42
2:F:176:GLU:HG3	2:F:224:LEU:HD21	2.02	0.41
2:F:134:LYS:H	2:F:134:LYS:HD3	1.85	0.41
1:A:484:ARG:HD2	1:A:614:TYR:OH	2.20	0.41
2:G:139:ASN:HD22	2:G:140:TYR:N	2.18	0.41
1:D:597:LEU:O	1:D:638:SER:HA	2.20	0.41
2:G:188:TRP:HA	2:G:200:HIS:O	2.20	0.41
2:H:132:LYS:HE3	2:H:132:LYS:HA	2.03	0.41
2:H:104:LEU:HG	2:H:105:LYS:HG2	2.03	0.41
1:A:509:LYS:HD3	1:A:509:LYS:HA	1.83	0.41
1:A:504:MET:HE2	1:A:504:MET:HB3	1.94	0.41
1:A:465:THR:HB	1:A:554:TYR:CZ	2.56	0.41
2:G:218:TYR:HB3	2:G:241:ILE:HD11	2.03	0.41
2:G:222:ALA:O	2:G:226:VAL:HG23	2.21	0.41
2:F:139:ASN:HA	2:F:163:LYS:HE3	2.03	0.40
2:E:108:ILE:HA	2:E:109:PRO:C	2.40	0.40
1:A:559:ASN:HD21	2:F:104:LEU:H	1.69	0.40
1:D:518:ILE:H	1:D:518:ILE:HD12	1.86	0.40
2:E:202:GLU:HG3	2:E:204:ARG:HG3	2.03	0.40
1:A:552:ALA:O	1:A:559:ASN:HA	2.22	0.40
1:C:469:THR:HB	1:C:470:PRO:HD2	2.04	0.40
1:B:493:LEU:HA	1:B:494:PRO:HD3	1.94	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	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
1	B	211/214 (99%)	207 (98%)	2 (1%)	2 (1%)	25	21
1	C	211/214 (99%)	206 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
2	E	138/150 (92%)	136 (99%)	2 (1%)	0	100	100
2	F	126/150 (84%)	118 (94%)	7 (6%)	1 (1%)	27	24
2	G	128/150 (85%)	122 (95%)	6 (5%)	0	100	100
2	H	136/150 (91%)	128 (94%)	7 (5%)	1 (1%)	30	28
All	All	1373/1456 (94%)	1331 (97%)	38 (3%)	4 (0%)	50	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	509	LYS
1	B	508	ARG
2	F	198	SER
2	H	118	ALA

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	186/186 (100%)	177 (95%)	9 (5%)	35	41
1	B	185/186 (100%)	182 (98%)	3 (2%)	75	85
1	C	185/186 (100%)	182 (98%)	3 (2%)	75	85
1	D	185/186 (100%)	181 (98%)	4 (2%)	64	76
2	E	128/133 (96%)	119 (93%)	9 (7%)	21	22
2	F	119/133 (90%)	110 (92%)	9 (8%)	19	18
2	G	120/133 (90%)	112 (93%)	8 (7%)	23	24
2	H	126/133 (95%)	118 (94%)	8 (6%)	25	27
All	All	1234/1276 (97%)	1181 (96%)	53 (4%)	40	47

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	ARG
1	A	507	LYS
1	A	508	ARG
1	A	560	LYS
1	A	571	GLN
1	A	595	VAL
1	A	600	SER
1	A	622	SER
1	A	664	GLU
1	B	508	ARG
1	B	564	THR
1	B	625	GLU
1	C	564	THR
1	C	571	GLN
1	C	604	ASP
1	D	489	ARG
1	D	595	VAL
1	D	620	SER
1	D	672	ARG
2	E	102	LEU
2	E	116	ASN
2	E	119	SER
2	E	130	SER
2	E	132	LYS
2	E	139	ASN
2	E	165	LYS
2	E	235	TYR
2	E	248	ASP
2	F	99	LEU
2	F	107	THR
2	F	111	LEU
2	F	138	PRO
2	F	139	ASN
2	F	157	LEU
2	F	160	LYS
2	F	181	ARG
2	F	235	TYR
2	G	103	VAL
2	G	112	SER
2	G	135	ASP
2	G	139	ASN
2	G	156	ARG
2	G	181	ARG

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Mol	Chain	Res	Type
2	G	197	GLU
2	G	235	TYR
2	H	116	ASN
2	H	129	ASP
2	H	132	LYS
2	H	134	LYS
2	H	135	ASP
2	H	139	ASN
2	H	180	ILE
2	H	235	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	ASN
1	A	544	HIS
1	A	563	ASN
1	A	571	GLN
1	A	598	HIS
1	A	670	GLN
1	B	501	GLN
1	B	559	ASN
1	B	598	HIS
1	B	635	HIS
1	B	670	GLN
1	C	510	ASN
1	C	559	ASN
1	C	571	GLN
1	C	598	HIS
1	D	510	ASN
1	D	517	ASN
1	D	670	GLN
2	E	139	ASN
2	E	193	HIS
2	F	139	ASN
2	F	240	HIS
2	G	139	ASN
2	G	193	HIS
2	H	139	ASN
2	H	175	ASN
2	H	215	GLN

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 ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	403	-	4,4,4	3.15	1 (25%)	6,6,6	0.37	0
3	PO4	A	404	-	4,4,4	3.27	1 (25%)	6,6,6	0.32	0
3	PO4	B	401	-	4,4,4	2.87	1 (25%)	6,6,6	0.34	0
3	PO4	B	406	-	4,4,4	3.29	1 (25%)	6,6,6	0.33	0
3	PO4	C	402	-	4,4,4	2.97	1 (25%)	6,6,6	0.36	0
3	PO4	C	407	-	4,4,4	3.24	1 (25%)	6,6,6	0.33	0
3	PO4	D	405	-	4,4,4	3.30	1 (25%)	6,6,6	0.33	0
3	PO4	E	408	-	4,4,4	3.26	1 (25%)	6,6,6	0.33	0
3	PO4	E	411	-	4,4,4	3.26	1 (25%)	6,6,6	0.34	0
3	PO4	E	412	-	4,4,4	3.29	1 (25%)	6,6,6	0.35	0
3	PO4	F	410	-	4,4,4	3.31	1 (25%)	6,6,6	0.33	0
3	PO4	H	409	-	4,4,4	3.28	1 (25%)	6,6,6	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	403	-	-	0/0/0/0	0/0/0/0
3	PO4	A	404	-	-	0/0/0/0	0/0/0/0
3	PO4	B	401	-	-	0/0/0/0	0/0/0/0
3	PO4	B	406	-	-	0/0/0/0	0/0/0/0
3	PO4	C	402	-	-	0/0/0/0	0/0/0/0
3	PO4	C	407	-	-	0/0/0/0	0/0/0/0
3	PO4	D	405	-	-	0/0/0/0	0/0/0/0
3	PO4	E	408	-	-	0/0/0/0	0/0/0/0
3	PO4	E	411	-	-	0/0/0/0	0/0/0/0
3	PO4	E	412	-	-	0/0/0/0	0/0/0/0
3	PO4	F	410	-	-	0/0/0/0	0/0/0/0
3	PO4	H	409	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	410	PO4	P-O4	6.61	1.79	1.52
3	D	405	PO4	P-O4	6.57	1.79	1.52
3	E	412	PO4	P-O4	6.57	1.79	1.52
3	H	409	PO4	P-O4	6.56	1.79	1.52
3	B	406	PO4	P-O4	6.55	1.79	1.52
3	A	404	PO4	P-O4	6.52	1.79	1.52
3	E	408	PO4	P-O4	6.51	1.79	1.52
3	E	411	PO4	P-O4	6.51	1.79	1.52
3	C	407	PO4	P-O4	6.47	1.78	1.52
3	A	403	PO4	P-O4	6.27	1.78	1.52
3	C	402	PO4	P-O4	5.91	1.76	1.52
3	B	401	PO4	P-O4	5.72	1.75	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	214/214 (100%)	0.06	2 (0%) 81 82	21, 30, 43, 54	0
1	B	213/214 (99%)	0.04	2 (0%) 81 82	24, 32, 45, 61	0
1	C	213/214 (99%)	0.07	3 (1%) 72 72	24, 32, 45, 58	0
1	D	213/214 (99%)	0.02	1 (0%) 88 90	24, 33, 44, 58	0
2	E	142/150 (94%)	0.29	3 (2%) 60 61	35, 43, 52, 62	0
2	F	132/150 (88%)	1.37	32 (24%) 1 1	39, 51, 60, 65	0
2	G	134/150 (89%)	0.74	14 (10%) 7 6	39, 49, 55, 58	0
2	H	140/150 (93%)	0.82	12 (8%) 11 10	44, 54, 62, 64	0
All	All	1401/1456 (96%)	0.34	69 (4%) 28 28	21, 38, 56, 65	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	127	ARG	8.0
2	F	129	ASP	5.9
2	F	203	GLY	5.4
2	F	126	ILE	5.3
2	F	205	ALA	5.1
2	F	187	SER	4.4
2	F	245	VAL	4.4
1	B	507	LYS	4.2
2	F	200	HIS	3.9
1	B	506	GLY	3.7
2	H	126	ILE	3.7
2	H	142	ARG	3.6
2	F	232	TRP	3.5
2	H	192	TYR	3.5
2	E	147	ARG	3.4
2	F	125	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	129	ASP	3.2
2	F	136	LEU	3.2
2	G	157	LEU	3.2
2	F	201	TYR	3.1
2	G	125	VAL	3.1
2	G	232	TRP	3.0
2	F	119	SER	3.0
2	G	140	TYR	3.0
2	H	114	TYR	3.0
1	A	508	ARG	3.0
2	G	188	TRP	2.9
2	G	114	TYR	2.8
2	F	204	ARG	2.7
2	F	140	TYR	2.7
2	G	186	GLU	2.7
2	F	137	VAL	2.7
2	G	160	LYS	2.7
2	F	114	TYR	2.7
2	F	128	ARG	2.6
2	F	157	LEU	2.6
2	H	145	LEU	2.5
1	C	508	ARG	2.4
2	H	134	LYS	2.4
2	F	231	ASP	2.4
2	F	198	SER	2.4
2	F	161	ARG	2.3
2	F	124	GLY	2.3
1	D	508	ARG	2.3
2	F	228	ALA	2.3
2	F	132	LYS	2.3
2	G	192	TYR	2.3
2	F	159	SER	2.3
2	H	179	GLY	2.2
2	F	158	MET	2.2
2	H	177	TRP	2.2
2	G	133	PHE	2.2
2	H	194	HIS	2.2
2	F	99	LEU	2.2
2	G	136	LEU	2.2
1	C	604	ASP	2.1
2	G	189	ASP	2.1
2	F	199	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	605	ALA	2.1
2	F	123	GLU	2.1
2	F	160	LYS	2.1
2	E	129	ASP	2.1
1	C	505	VAL	2.1
2	G	201	TYR	2.1
2	E	134	LYS	2.1
2	H	138	PRO	2.1
2	H	100	TYR	2.1
2	G	196	GLN	2.0
2	F	134	LYS	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 ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	E	408	5/5	0.19	1.67	78,78,79,79	0
3	PO4	E	412	5/5	0.17	0.87	57,58,60,60	0
3	PO4	E	411	5/5	0.18	0.68	70,70,71,72	0
3	PO4	B	401	5/5	0.14	0.32	24,26,29,29	0
3	PO4	A	404	5/5	0.12	-0.66	68,69,69,69	0
3	PO4	B	406	5/5	0.08	-1.35	75,76,76,76	0
3	PO4	C	407	5/5	0.11	-1.50	79,79,79,80	0
3	PO4	D	405	5/5	0.11	-1.59	79,79,79,80	0
3	PO4	H	409	5/5	0.12	-1.72	76,77,78,78	0
3	PO4	A	403	5/5	0.12	-2.24	35,35,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	C	402	5/5	0.12	-2.70	29,30,31,32	0
3	PO4	F	410	5/5	0.11	-3.44	91,91,91,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.