



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:09 AM GMT

PDB ID : 3KE9  
Title : Crystal structure of IspH:Intermediate-complex  
Authors : Groll, M.; Graewert, T.; Span, I.; Eisenreich, W.; Bacher, A.  
Deposited on : 2009-10-24  
Resolution : 1.90 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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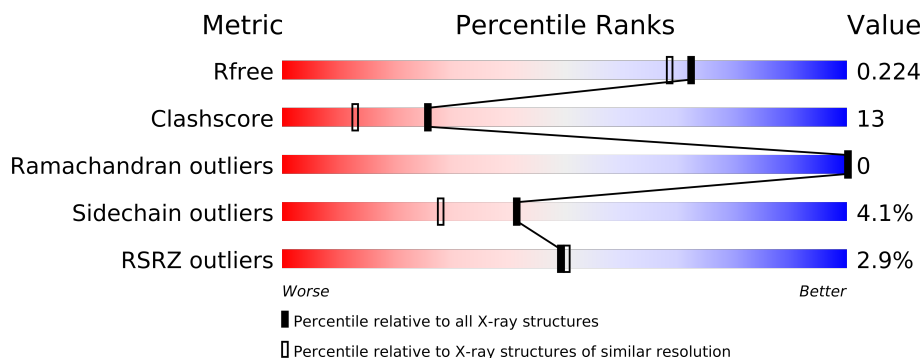
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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  $\geq 3$ , 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	326	
1	B	326	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5301 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 4-hydroxy-3-methylbut-2-enyldiphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2383	1487	427	459	10			
1	B	310	Total	C	N	O	S	0	0	0
			2390	1492	428	460	10			

There are 20 discrepancies between the modelled and reference sequences:

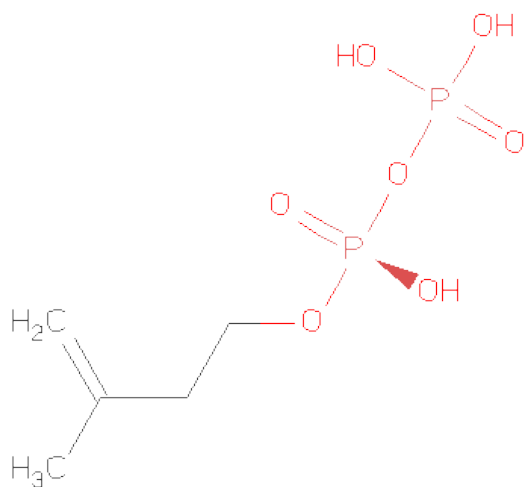
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP P62623
A	-8	ARG	-	EXPRESSION TAG	UNP P62623
A	-7	GLY	-	EXPRESSION TAG	UNP P62623
A	-6	SER	-	EXPRESSION TAG	UNP P62623
A	-5	HIS	-	EXPRESSION TAG	UNP P62623
A	-4	HIS	-	EXPRESSION TAG	UNP P62623
A	-3	HIS	-	EXPRESSION TAG	UNP P62623
A	-2	HIS	-	EXPRESSION TAG	UNP P62623
A	-1	HIS	-	EXPRESSION TAG	UNP P62623
A	0	HIS	-	EXPRESSION TAG	UNP P62623
B	-9	MET	-	EXPRESSION TAG	UNP P62623
B	-8	ARG	-	EXPRESSION TAG	UNP P62623
B	-7	GLY	-	EXPRESSION TAG	UNP P62623
B	-6	SER	-	EXPRESSION TAG	UNP P62623
B	-5	HIS	-	EXPRESSION TAG	UNP P62623
B	-4	HIS	-	EXPRESSION TAG	UNP P62623
B	-3	HIS	-	EXPRESSION TAG	UNP P62623
B	-2	HIS	-	EXPRESSION TAG	UNP P62623
B	-1	HIS	-	EXPRESSION TAG	UNP P62623
B	0	HIS	-	EXPRESSION TAG	UNP P62623

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula:  $C_5H_{12}O_7P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	7	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 4 is water.

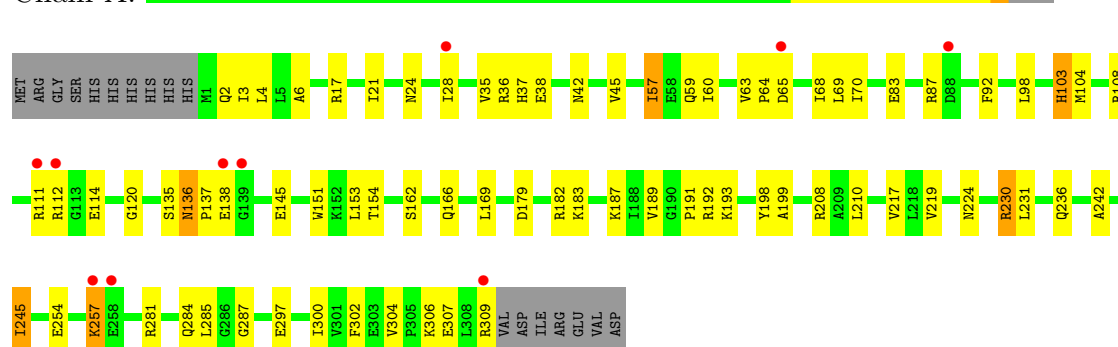
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		
4	B	254	Total	O	0	0
			254	254		

### 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.

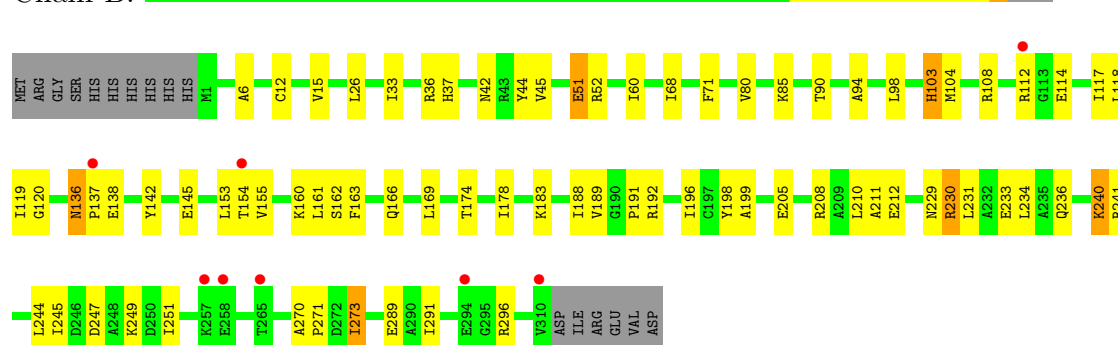
- Molecule 1: 4-hydroxy-3-methylbut-2-enyldiphosphate reductase

Chain A:



- Molecule 1: 4-hydroxy-3-methylbut-2-enyldiphosphate reductase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.61Å 80.83Å 112.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 24.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-1.90) 99.9 (24.85-1.80)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 1.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.214 , 0.248 0.220 , 0.224	Depositor DCC
$R_{free}$ test set	2977 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59528 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5301	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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 44.15 % 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 1.5917e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, IPE

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	0.28	0/2418	0.56	0/3273
1	B	0.29	0/2425	0.57	0/3283
All	All	0.29	0/4843	0.57	0/6556

There are no bond length outliers.

There are no bond angle outliers.

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	2383	0	2395	65	0
1	B	2390	0	2404	67	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	14	0	9	0	0
3	B	14	0	9	0	0
4	A	230	0	0	5	0
4	B	254	0	0	7	0
All	All	5301	0	4817	130	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 13.

All (130) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:120:GLY:O	1:B:145:GLU:HG2	1.77	0.85
1:B:296:ARG:HB2	1:B:296:ARG:HH21	1.43	0.83
1:A:120:GLY:O	1:A:145:GLU:HG2	1.78	0.82
1:A:42:ASN:HD22	1:A:45:VAL:H	1.25	0.81
1:A:24:ASN:O	1:A:28:ILE:HG12	1.83	0.77
1:A:187:LYS:HA	1:A:187:LYS:HE2	1.66	0.77
1:A:57:ILE:HD13	1:A:57:ILE:H	1.53	0.74
1:B:42:ASN:HD22	1:B:45:VAL:H	1.36	0.74
1:B:296:ARG:HB2	1:B:296:ARG:NH2	2.03	0.72
1:B:117:ILE:HD12	1:B:153:LEU:HD11	1.72	0.72
1:A:236:GLN:HG3	1:A:242:ALA:HB3	1.76	0.68
1:B:174:THR:O	1:B:178:ILE:HG12	1.94	0.68
1:A:245:ILE:HD13	1:A:245:ILE:H	1.58	0.68
1:B:136:ASN:HD22	1:B:137:PRO:N	1.93	0.67
1:A:17:ARG:O	1:A:21:ILE:HD13	1.94	0.66
1:A:306:LYS:O	1:A:309:ARG:HG2	1.95	0.66
1:A:281:ARG:HH21	1:A:284:GLN:HG3	1.61	0.66
1:A:257:LYS:HD2	1:A:257:LYS:O	1.95	0.65
1:B:245:ILE:HD13	1:B:251:ILE:HD11	1.79	0.65
1:B:51:GLU:HG3	1:B:52:ARG:HD2	1.79	0.65
1:A:21:ILE:HD12	1:A:304:VAL:HG12	1.78	0.65
1:A:153:LEU:HD23	1:A:154:THR:N	2.12	0.65
1:B:296:ARG:CB	1:B:296:ARG:HH21	2.11	0.63
1:B:68:ILE:HD13	1:B:90:THR:HB	1.81	0.63
1:A:2:GLN:NE2	1:A:4:LEU:HD11	2.15	0.61
1:A:254:GLU:O	1:A:257:LYS:HG3	2.00	0.61
1:B:136:ASN:ND2	1:B:138:GLU:H	1.99	0.60
1:B:249:LYS:HE2	1:B:249:LYS:H	1.66	0.60
1:A:59:GLN:HB3	4:A:620:HOH:O	2.00	0.60
1:A:192:ARG:NH2	1:B:191:PRO:HD3	2.16	0.60
1:B:273:ILE:O	1:B:273:ILE:HD13	2.01	0.59
1:B:161:LEU:O	1:B:189:VAL:HG12	2.02	0.59
1:B:114:GLU:OE1	1:B:160:LYS:HB3	2.03	0.59
1:B:117:ILE:CD1	1:B:153:LEU:HD11	2.33	0.59
1:B:169:LEU:HB2	1:B:196:ILE:HD11	1.85	0.58
1:B:6:ALA:HB2	1:B:210:LEU:HD22	1.85	0.57
1:B:153:LEU:HD23	1:B:154:THR:N	2.20	0.56
1:B:42:ASN:HD21	1:B:44:TYR:HB3	1.71	0.56
1:A:38:GLU:OE2	1:A:224:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300:ILE:HD11	1:A:302:PHE:CE2	2.41	0.56
1:B:136:ASN:C	1:B:136:ASN:HD22	2.06	0.56
1:B:245:ILE:CD1	1:B:251:ILE:HD11	2.35	0.55
1:B:205:GLU:HA	1:B:208:ARG:NH2	2.20	0.55
1:A:245:ILE:HD13	1:A:245:ILE:N	2.20	0.55
1:B:153:LEU:HD22	1:B:155:VAL:HG23	1.89	0.54
1:B:112:ARG:HG3	1:B:112:ARG:HH21	1.71	0.54
1:A:68:ILE:HD12	1:A:68:ILE:N	2.22	0.54
1:A:112:ARG:O	1:A:114:GLU:HG3	2.08	0.53
1:B:166:GLN:O	1:B:196:ILE:HD13	2.09	0.53
1:B:119:ILE:HD12	1:B:119:ILE:N	2.23	0.53
1:B:136:ASN:HD22	1:B:137:PRO:CD	2.22	0.53
1:A:281:ARG:HD3	4:A:571:HOH:O	2.09	0.53
1:B:205:GLU:HG3	4:B:321:HOH:O	2.08	0.52
1:B:236:GLN:HG2	4:B:587:HOH:O	2.09	0.52
1:A:179:ASP:O	1:A:183:LYS:HG3	2.10	0.51
1:A:2:GLN:HG2	1:A:4:LEU:CD1	2.40	0.51
1:A:36:ARG:O	1:A:37:HIS:HB2	2.11	0.51
1:A:2:GLN:C	1:A:3:ILE:HD12	2.30	0.51
1:A:42:ASN:ND2	1:A:45:VAL:H	2.03	0.51
1:B:51:GLU:HG2	4:B:705:HOH:O	2.10	0.51
1:B:108:ARG:HH21	1:B:108:ARG:HG3	1.74	0.51
1:B:205:GLU:HA	1:B:208:ARG:HH22	1.74	0.51
1:A:191:PRO:HD3	1:B:192:ARG:NH2	2.26	0.51
1:B:117:ILE:CD1	1:B:142:TYR:HB2	2.41	0.50
1:B:183:LYS:HG3	4:B:361:HOH:O	2.11	0.50
1:A:193:LYS:HA	4:A:684:HOH:O	2.11	0.50
1:A:60:ILE:HB	1:A:83:GLU:OE2	2.11	0.49
1:A:3:ILE:HD12	1:A:3:ILE:N	2.27	0.49
1:A:35:VAL:O	1:A:57:ILE:HD13	2.12	0.49
1:A:135:SER:O	1:A:137:PRO:HD3	2.12	0.49
1:B:166:GLN:HB3	1:B:169:LEU:HG	1.94	0.48
1:A:57:ILE:N	1:A:57:ILE:HD13	2.25	0.48
1:B:163:PHE:CE1	1:B:178:ILE:HD12	2.48	0.48
1:A:136:ASN:ND2	1:A:138:GLU:H	2.11	0.48
1:B:36:ARG:O	1:B:37:HIS:HB2	2.14	0.48
1:B:291:ILE:HD12	1:B:291:ILE:N	2.29	0.47
1:A:3:ILE:HD11	1:A:287:GLY:HA3	1.95	0.47
1:A:21:ILE:CD1	1:A:304:VAL:HG12	2.43	0.47
1:A:104:MET:CE	1:A:104:MET:HA	2.44	0.47
1:A:182:ARG:HH21	1:A:182:ARG:HG3	1.80	0.47
1:B:103:HIS:HD2	4:B:515:HOH:O	1.98	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:LEU:HD23	1:B:33:ILE:HG12	1.96	0.47
1:A:17:ARG:HD2	1:A:302:PHE:HB3	1.95	0.47
1:B:198:TYR:CG	1:B:199:ALA:N	2.83	0.47
1:A:2:GLN:HE21	1:A:4:LEU:HD11	1.77	0.46
1:A:281:ARG:O	1:A:284:GLN:HG2	2.15	0.46
1:B:163:PHE:HB3	1:B:188:ILE:HD11	1.98	0.46
1:A:136:ASN:HD22	1:A:136:ASN:C	2.19	0.46
1:B:229:ASN:O	1:B:233:GLU:HG3	2.15	0.46
1:A:219:VAL:O	1:A:245:ILE:HD13	2.16	0.46
1:A:21:ILE:HD12	1:A:304:VAL:CG1	2.45	0.45
1:B:208:ARG:O	1:B:212:GLU:HG3	2.17	0.45
1:A:162:SER:HA	1:A:189:VAL:O	2.16	0.45
1:B:230:ARG:HD3	1:B:230:ARG:HA	1.77	0.45
1:B:289:GLU:O	1:B:291:ILE:HD12	2.16	0.44
1:A:63:VAL:O	1:A:87:ARG:NH2	2.48	0.44
1:A:166:GLN:HB3	1:A:169:LEU:HG	1.99	0.44
1:A:306:LYS:HG3	1:A:307:GLU:N	2.31	0.44
1:A:6:ALA:HB2	1:A:210:LEU:HD22	2.00	0.44
1:B:162:SER:HA	1:B:189:VAL:O	2.18	0.44
1:B:211:ALA:O	1:B:240:LYS:NZ	2.47	0.43
1:A:108:ARG:HA	1:A:111:ARG:NH1	2.33	0.43
1:B:234:LEU:HD23	1:B:234:LEU:O	2.18	0.43
1:B:247:ASP:OD1	1:B:249:LYS:HB2	2.19	0.43
1:B:68:ILE:CD1	1:B:90:THR:HB	2.49	0.43
1:A:70:ILE:HG12	1:A:92:PHE:HB2	2.00	0.43
1:B:270:ALA:HA	1:B:271:PRO:HD3	1.85	0.43
1:A:230:ARG:HD3	1:A:230:ARG:HA	1.72	0.43
1:B:71:PHE:O	1:B:94:ALA:HB3	2.18	0.43
1:A:198:TYR:CG	1:A:199:ALA:N	2.86	0.42
1:B:136:ASN:ND2	1:B:136:ASN:C	2.72	0.42
1:B:234:LEU:HD23	1:B:234:LEU:C	2.39	0.42
1:A:208:ARG:HB2	1:A:208:ARG:NH2	2.34	0.42
1:B:85:LYS:HB3	1:B:85:LYS:HE2	1.89	0.42
1:B:12:CYS:SG	1:B:15:VAL:HG23	2.60	0.42
1:A:217:VAL:O	1:A:242:ALA:HA	2.20	0.41
1:B:60:ILE:HD11	1:B:80:VAL:HG13	2.01	0.41
1:A:104:MET:HE2	1:A:104:MET:HA	2.02	0.41
1:B:155:VAL:HG21	1:B:161:LEU:HD11	2.02	0.41
1:A:257:LYS:O	1:A:257:LYS:CD	2.66	0.41
1:A:297:GLU:HG3	4:A:536:HOH:O	2.20	0.41
1:B:240:LYS:N	1:B:240:LYS:HD2	2.35	0.41
1:B:108:ARG:CZ	1:B:108:ARG:HB2	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:VAL:HA	1:A:64:PRO:HD3	1.87	0.41
1:A:151:TRP:HE3	1:A:151:TRP:HA	1.85	0.40
1:A:300:ILE:HD11	1:A:302:PHE:CZ	2.56	0.40
1:A:103:HIS:HD2	4:A:384:HOH:O	2.04	0.40
1:B:241:ARG:HG3	4:B:559:HOH:O	2.22	0.40
1:B:104:MET:CE	4:B:682:HOH:O	2.69	0.40
1:A:151:TRP:CE3	1:A:151:TRP:HA	2.56	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	307/326 (94%)	302 (98%)	5 (2%)	0	100	100
1	B	308/326 (94%)	304 (99%)	4 (1%)	0	100	100
All	All	615/652 (94%)	606 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	257/273 (94%)	246 (96%)	11 (4%)	40	26
1	B	258/273 (94%)	248 (96%)	10 (4%)	43	30
All	All	515/546 (94%)	494 (96%)	21 (4%)	41	28

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	65	ASP
1	A	69	LEU
1	A	98	LEU
1	A	103	HIS
1	A	136	ASN
1	A	230	ARG
1	A	231	LEU
1	A	245	ILE
1	A	257	LYS
1	A	285	LEU
1	B	51	GLU
1	B	98	LEU
1	B	103	HIS
1	B	118	LEU
1	B	136	ASN
1	B	230	ARG
1	B	231	LEU
1	B	240	LYS
1	B	244	LEU
1	B	273	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	42	ASN
1	A	59	GLN
1	A	78	GLN
1	A	103	HIS
1	A	133	GLN
1	A	136	ASN
1	A	229	ASN
1	A	236	GLN
1	A	252	GLN
1	A	277	ASN
1	A	283	GLN
1	B	2	GLN
1	B	37	HIS
1	B	42	ASN
1	B	78	GLN
1	B	103	HIS
1	B	133	GLN

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Mol	Chain	Res	Type
1	B	136	ASN
1	B	229	ASN
1	B	277	ASN
1	B	283	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 ⓘ

4 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	$\# Z  > 2$
2	SF4	A	997	1	12,12,12	12.17	12 (100%)	0,24,24	0.00	-
3	IPE	A	998	-	13,13,13	1.92	2 (15%)	19,19,19	2.34	6 (31%)
2	SF4	B	997	1	12,12,12	12.05	11 (91%)	0,24,24	0.00	-
3	IPE	B	998	-	13,13,13	1.89	2 (15%)	19,19,19	2.30	6 (31%)

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
2	SF4	A	997	1	-	0/0/48/48	0/0/5/5
3	IPE	A	998	-	-	1/13/13/13	0/0/0/0
2	SF4	B	997	1	-	0/0/48/48	0/0/5/5
3	IPE	B	998	-	-	1/13/13/13	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	SF4	S3-FE2	-21.25	2.19	2.33
2	B	997	SF4	S4-FE2	-20.36	2.19	2.33
2	A	997	SF4	S4-FE2	-20.34	2.19	2.33
2	B	997	SF4	S3-FE2	-20.19	2.19	2.33
2	B	997	SF4	S1-FE2	-16.45	2.22	2.33
2	A	997	SF4	S2-FE1	-16.29	2.22	2.33
2	A	997	SF4	S1-FE2	-16.05	2.22	2.33
2	B	997	SF4	S2-FE1	-14.99	2.23	2.33
2	B	997	SF4	S3-FE4	13.55	2.42	2.33
2	A	997	SF4	S3-FE4	12.65	2.41	2.33
2	A	997	SF4	S4-FE1	-9.59	2.26	2.33
2	B	997	SF4	S4-FE1	-9.24	2.27	2.33
2	B	997	SF4	S1-FE4	7.00	2.38	2.33
2	B	997	SF4	S2-FE4	6.77	2.37	2.33
2	B	997	SF4	S2-FE3	-6.58	2.28	2.33
2	A	997	SF4	S2-FE4	6.29	2.37	2.33
2	A	997	SF4	S2-FE3	-6.18	2.29	2.33
2	A	997	SF4	S1-FE4	5.88	2.37	2.33
3	A	998	IPE	C4-C3	5.20	1.50	1.33
3	B	998	IPE	C4-C3	5.18	1.50	1.33
3	B	998	IPE	C2-C3	-3.32	1.43	1.51
2	B	997	SF4	S4-FE3	-3.14	2.31	2.33
2	A	997	SF4	S3-FE1	-3.03	2.31	2.33
3	A	998	IPE	C2-C3	-2.98	1.44	1.51
2	A	997	SF4	S1-FE3	-2.73	2.31	2.33
2	B	997	SF4	S1-FE3	-2.70	2.31	2.33
2	A	997	SF4	S4-FE3	-2.70	2.31	2.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	IPE	O3A-PA-O1	6.53	132.62	103.41
3	B	998	IPE	O3A-PA-O1	6.44	132.22	103.41
3	A	998	IPE	O2A-PA-O1	-4.69	84.87	108.51
3	B	998	IPE	O2A-PA-O1	-4.66	85.02	108.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	IPE	PA-O3A-PB	-3.83	120.46	131.68
3	B	998	IPE	PA-O3A-PB	-3.76	120.65	131.68
3	A	998	IPE	C1-C2-C3	2.92	126.11	111.80
3	B	998	IPE	C1-C2-C3	2.77	125.40	111.80
3	B	998	IPE	O1B-PB-O3A	2.17	115.43	105.14
3	A	998	IPE	O1B-PB-O3A	2.11	115.14	105.14
3	A	998	IPE	PA-O1-C1	2.10	133.50	121.66
3	B	998	IPE	PA-O1-C1	2.02	133.03	121.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	998	IPE	PA-O1-C1-C2
3	B	998	IPE	PA-O1-C1-C2

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, 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	309/326 (94%)	0.31	10 (3%) 45 46	21, 34, 53, 58	0
1	B	310/326 (95%)	0.23	8 (2%) 53 55	20, 33, 49, 59	0
All	All	619/652 (94%)	0.27	18 (2%) 49 50	20, 34, 51, 59	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	ASP	3.8
1	A	258	GLU	2.8
1	B	112	ARG	2.7
1	B	310	VAL	2.7
1	A	309	ARG	2.7
1	A	138	GLU	2.6
1	B	258	GLU	2.4
1	A	65	ASP	2.4
1	A	112	ARG	2.3
1	A	111	ARG	2.2
1	A	28	ILE	2.2
1	B	137	PRO	2.2
1	B	294	GLU	2.1
1	B	154	THR	2.1
1	A	257	LYS	2.1
1	B	265	THR	2.1
1	B	257	LYS	2.0
1	A	139	GLY	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	IPE	A	998	14/14	0.16	1.39	21,24,26,29	0
3	IPE	B	998	14/14	0.12	0.69	19,23,26,27	0
2	SF4	B	997	8/8	0.08	-0.95	25,26,28,31	0
2	SF4	A	997	8/8	0.08	-1.04	26,28,28,31	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.