



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:58 AM UTC

PDB ID : 3KEM / pdb_00003kem
Title : Crystal structure of IspH:IPP complex
Authors : Groll, M.; Graewert, T.; Span, I.; Eisenreich, W.; Bacher, A.
Deposited on : 2009-10-26
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

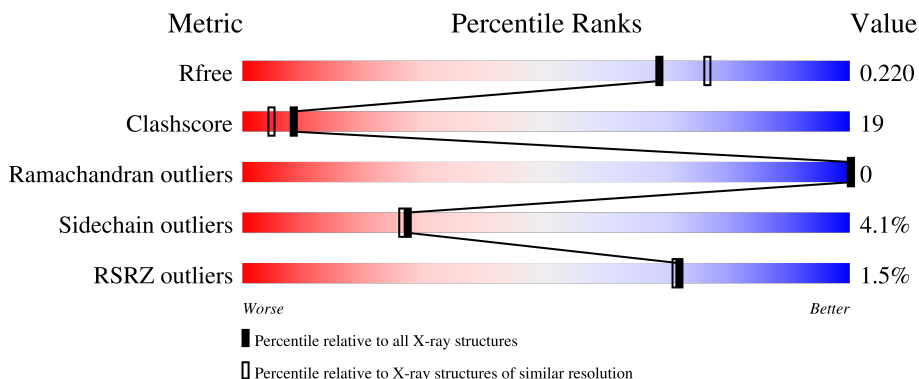
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

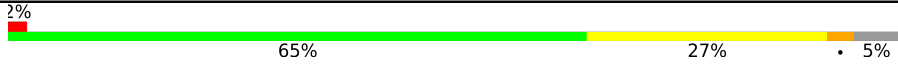
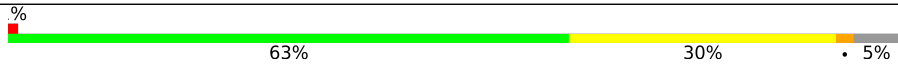
The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	326	
1	B	326	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5269 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.

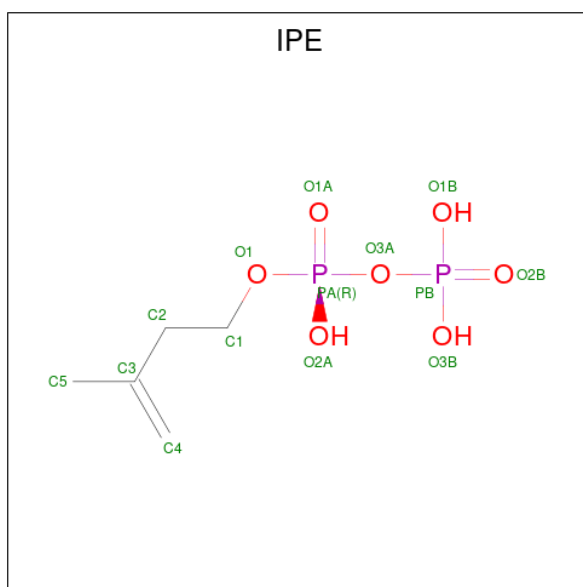
- Molecule 1 is a protein called 4-hydroxy-3-methylbut-2-enyl diphosphate reductase.

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:

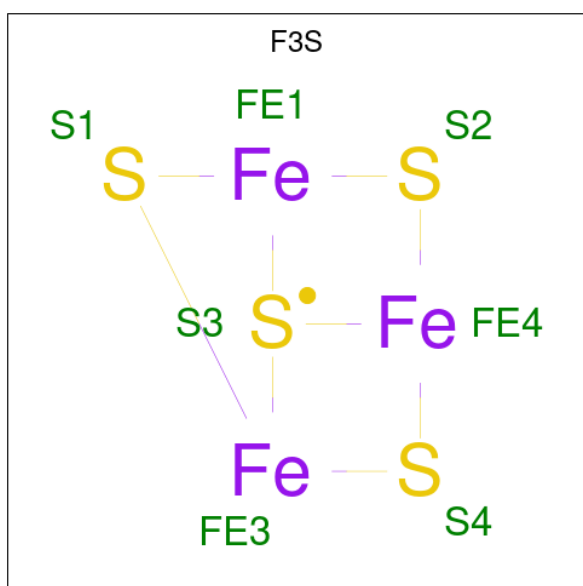
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP P62623
A	-8	ARG	-	expression tag	UNP P62623
A	-7	GLY	-	expression tag	UNP P62623
A	-6	SER	-	expression tag	UNP P62623
A	-5	HIS	-	expression tag	UNP P62623
A	-4	HIS	-	expression tag	UNP P62623
A	-3	HIS	-	expression tag	UNP P62623
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 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (CCD ID: IPE) (formula: $C_5H_{12}O_7P_2$).



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

- Molecule 3 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		
3	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total 220	O 220	0	0
4	B	234	Total 234	O 234	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.47Å 80.64Å 70.16Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	9.99 – 2.00 9.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.4 (9.99-2.00) 93.7 (9.99-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.275 0.223 , 0.220	Depositor DCC
R_{free} test set	2017 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5269	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPE, F3S

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/2418	0.87	6/3273 (0.2%)
1	B	0.38	0/2425	0.89	5/3283 (0.2%)
All	All	0.37	0/4843	0.88	11/6556 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	GLN	N-CA-C	-6.65	101.12	110.50
1	B	11	PHE	N-CA-C	6.24	119.53	110.42
1	A	166	GLN	N-CA-C	-5.97	102.08	110.50
1	A	284	GLN	N-CA-C	-5.92	106.11	113.15
1	B	136	ASN	CA-C-N	5.68	125.36	119.05
1	B	136	ASN	C-N-CA	5.68	125.36	119.05
1	A	12	CYS	N-CA-C	-5.56	102.23	110.46
1	A	11	PHE	N-CA-C	5.35	118.56	110.64
1	A	91	VAL	N-CA-C	5.34	116.27	108.53
1	A	99	VAL	N-CA-C	-5.17	106.10	111.58
1	B	99	VAL	N-CA-C	-5.04	105.93	110.82

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	2383	0	2395	88	0
1	B	2390	0	2404	96	0
2	A	14	0	9	0	0
2	B	14	0	9	0	0
3	A	7	0	0	0	0
3	B	7	0	0	1	0
4	A	220	0	0	13	0
4	B	234	0	0	12	0
All	All	5269	0	4817	184	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 19.

All (184) 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:B:120:GLY:O	1:B:145:GLU:HG2	1.79	0.82
1:A:248:ALA:HB2	4:A:394:HOH:O	1.79	0.81
1:B:21:ILE:HG12	1:B:304:VAL:HG13	1.63	0.80
1:A:117:ILE:HG12	1:A:161:LEU:HD21	1.62	0.79
1:A:236:GLN:HG3	1:A:242:ALA:HB3	1.62	0.78
1:B:257:LYS:HG2	1:B:258:GLU:HG3	1.65	0.78
1:A:117:ILE:HD12	1:A:153:LEU:HD11	1.64	0.78
1:B:104:MET:HA	1:B:104:MET:HE2	1.64	0.77
1:B:248:ALA:HA	1:B:251:ILE:HD13	1.68	0.74
1:B:7:ASN:HD22	1:B:8:PRO:HA	1.54	0.72
1:B:245:ILE:H	1:B:245:ILE:HD13	1.55	0.72
1:A:304:VAL:HG13	1:A:305:PRO:HD2	1.71	0.72
1:B:68:ILE:HD13	1:B:90:THR:HB	1.71	0.71
1:B:39:VAL:HA	4:B:385:HOH:O	1.90	0.71
1:B:24:ASN:O	1:B:28:ILE:HG12	1.91	0.71
1:A:120:GLY:O	1:A:145:GLU:HG2	1.90	0.71
1:B:37:HIS:HE1	1:B:41:HIS:NE2	1.88	0.70
1:B:117:ILE:HD12	1:B:153:LEU:HD11	1.73	0.70
1:A:42:ASN:HD22	1:A:45:VAL:H	1.41	0.68
1:A:161:LEU:HD23	1:A:162:SER:N	2.10	0.66
1:B:42:ASN:HD22	1:B:45:VAL:H	1.42	0.66
1:A:201:THR:O	1:A:205:GLU:HG3	1.95	0.66
1:B:208:ARG:O	1:B:212:GLU:HG2	1.96	0.66
1:B:115:GLU:CD	1:B:155:VAL:HG22	2.22	0.65
1:A:281:ARG:HH21	1:A:284:GLN:HG3	1.62	0.63
1:A:248:ALA:HA	1:A:251:ILE:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASP:CG	1:B:196:ILE:HD13	2.22	0.63
1:B:28:ILE:HD11	1:B:310:VAL:HG22	1.81	0.63
1:B:2:GLN:HG2	1:B:4:LEU:HD13	1.80	0.63
1:A:161:LEU:HD22	1:A:188:ILE:HG13	1.81	0.62
1:B:153:LEU:HD23	1:B:154:THR:N	2.15	0.62
1:A:240:LYS:N	1:A:240:LYS:HD2	2.15	0.62
1:B:174:THR:O	1:B:178:ILE:HG12	2.00	0.62
1:B:70:ILE:CD1	1:B:92:PHE:HB2	2.30	0.61
1:B:281:ARG:HH21	1:B:284:GLN:HG3	1.64	0.60
1:A:174:THR:O	1:A:178:ILE:HG12	2.01	0.60
1:B:245:ILE:HD13	1:B:245:ILE:N	2.17	0.60
1:A:273:ILE:HD13	1:A:273:ILE:O	2.02	0.59
1:A:70:ILE:HD13	1:A:92:PHE:HB2	1.84	0.59
1:A:281:ARG:HH21	1:A:284:GLN:CG	2.15	0.58
1:B:70:ILE:HD13	1:B:92:PHE:HB2	1.85	0.58
1:A:306:LYS:O	1:A:309:ARG:HG2	2.03	0.58
1:A:118:LEU:HD12	1:A:131:MET:HG3	1.85	0.57
1:B:251:ILE:HD12	1:B:251:ILE:N	2.20	0.57
1:B:108:ARG:HD3	4:B:420:HOH:O	2.06	0.56
1:B:221:GLY:O	1:B:244:LEU:HD22	2.04	0.56
1:A:166:GLN:HB3	1:A:169:LEU:HG	1.87	0.56
1:A:211:ALA:C	1:A:213:GLN:H	2.13	0.56
1:B:7:ASN:HD22	1:B:8:PRO:CA	2.19	0.55
1:A:209:ALA:HA	1:A:212:GLU:OE2	2.06	0.55
1:B:236:GLN:HG3	1:B:242:ALA:HB3	1.87	0.55
1:B:304:VAL:CG1	1:B:305:PRO:HD2	2.36	0.55
1:A:136:ASN:HD22	1:A:136:ASN:C	2.15	0.55
1:A:42:ASN:HD21	1:A:44:TYR:HB3	1.72	0.55
1:A:251:ILE:HD12	1:A:251:ILE:N	2.22	0.55
1:B:304:VAL:HG23	4:B:358:HOH:O	2.07	0.54
1:A:119:ILE:HD12	1:A:119:ILE:N	2.23	0.54
1:B:161:LEU:HD13	1:B:188:ILE:HD12	1.88	0.54
1:A:136:ASN:ND2	1:A:138:GLU:H	2.06	0.54
1:A:278:VAL:HG23	4:A:394:HOH:O	2.08	0.53
1:A:52:ARG:HG2	4:A:401:HOH:O	2.09	0.53
1:A:136:ASN:HD22	1:A:137:PRO:N	2.07	0.53
1:A:278:VAL:N	4:A:394:HOH:O	2.40	0.53
1:B:57:ILE:C	1:B:57:ILE:HD12	2.34	0.53
1:B:103:HIS:HD2	4:B:351:HOH:O	1.90	0.52
1:A:245:ILE:HD12	1:A:251:ILE:HD11	1.92	0.52
1:A:36:ARG:O	1:A:37:HIS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASN:C	1:B:136:ASN:HD22	2.18	0.52
1:A:275:VAL:HG21	4:A:369:HOH:O	2.09	0.52
1:A:161:LEU:HD22	1:A:188:ILE:CD1	2.41	0.52
1:B:35:VAL:HG12	4:B:385:HOH:O	2.09	0.51
1:B:196:ILE:HD12	1:B:196:ILE:N	2.26	0.51
1:A:294:GLU:HG3	4:A:481:HOH:O	2.10	0.51
1:B:136:ASN:HD22	1:B:137:PRO:CD	2.23	0.51
1:B:198:TYR:CG	1:B:199:ALA:N	2.79	0.51
1:B:205:GLU:CD	1:B:296:ARG:HH11	2.19	0.51
1:A:248:ALA:O	1:A:251:ILE:HD13	2.12	0.50
1:B:119:ILE:N	1:B:119:ILE:HD12	2.27	0.50
1:B:281:ARG:HH21	1:B:284:GLN:CG	2.25	0.50
1:B:2:GLN:HA	4:B:466:HOH:O	2.12	0.49
1:A:19:ILE:CD1	1:A:45:VAL:HG11	2.43	0.49
1:B:159:GLU:OE1	1:B:187:LYS:HD2	2.13	0.49
1:A:291:ILE:HD12	1:A:291:ILE:N	2.28	0.48
1:B:108:ARG:HG3	1:B:108:ARG:HH21	1.77	0.48
1:A:204:GLN:O	1:A:207:VAL:HG12	2.13	0.48
1:A:108:ARG:HH21	1:A:108:ARG:HG3	1.78	0.48
1:A:161:LEU:HD23	1:A:162:SER:H	1.76	0.48
1:B:72:SER:CB	4:B:385:HOH:O	2.62	0.48
1:A:153:LEU:HD23	1:A:154:THR:N	2.28	0.48
1:B:126:GLU:HB2	4:B:359:HOH:O	2.13	0.48
1:A:157:ASN:OD1	1:A:159:GLU:HB3	2.13	0.48
1:B:248:ALA:CA	1:B:251:ILE:HD13	2.41	0.47
1:A:163:PHE:CE1	1:A:178:ILE:HD12	2.49	0.47
1:B:2:GLN:NE2	1:B:4:LEU:HD11	2.29	0.47
1:A:281:ARG:O	1:A:285:LEU:HB2	2.14	0.47
1:A:283:GLN:C	1:A:285:LEU:H	2.22	0.47
1:A:58:GLU:HG3	4:A:490:HOH:O	2.14	0.47
1:A:71:PHE:O	1:A:94:ALA:HB3	2.14	0.47
1:A:234:LEU:HD23	1:A:234:LEU:O	2.13	0.47
1:B:21:ILE:CG1	1:B:304:VAL:HG13	2.41	0.47
1:B:81:ARG:HG2	1:B:85:LYS:HE3	1.97	0.47
1:B:136:ASN:HD22	1:B:137:PRO:N	2.12	0.47
1:A:151:TRP:HD1	4:A:359:HOH:O	1.97	0.47
1:A:241:ARG:NH1	1:A:255:TRP:O	2.46	0.47
1:A:211:ALA:C	1:A:213:GLN:N	2.73	0.47
1:A:19:ILE:HD12	1:A:45:VAL:HG11	1.96	0.47
1:B:57:ILE:HD13	1:B:59:GLN:O	2.15	0.46
1:A:257:LYS:HG2	1:A:258:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:HB3	4:B:385:HOH:O	2.15	0.46
1:B:162:SER:HA	1:B:189:VAL:O	2.16	0.46
1:A:161:LEU:HD22	1:A:188:ILE:CG1	2.46	0.46
1:B:300:ILE:HD11	4:B:355:HOH:O	2.16	0.46
1:B:4:LEU:HD22	1:B:261:CYS:SG	2.56	0.46
1:B:136:ASN:HD22	1:B:137:PRO:HD2	1.81	0.46
1:A:253:GLU:HG3	4:A:368:HOH:O	2.15	0.46
1:B:115:GLU:OE1	1:B:155:VAL:HG22	2.15	0.46
1:B:60:ILE:HD13	1:B:84:ALA:HB2	1.97	0.45
1:A:36:ARG:HH21	1:A:36:ARG:HG2	1.81	0.45
1:B:71:PHE:O	1:B:94:ALA:HB3	2.16	0.45
1:B:163:PHE:CZ	1:B:178:ILE:HD12	2.51	0.45
1:B:166:GLN:HB3	1:B:169:LEU:HG	1.99	0.45
1:A:112:ARG:NH1	4:A:516:HOH:O	2.48	0.45
1:A:119:ILE:HD13	1:A:165:THR:HG22	1.99	0.45
1:B:14:GLY:HA3	3:B:997:F3S:S4	2.57	0.45
1:A:15:VAL:O	1:A:19:ILE:HG12	2.17	0.44
1:B:35:VAL:CG1	4:B:385:HOH:O	2.64	0.44
1:B:281:ARG:HH21	1:B:284:GLN:CD	2.25	0.44
1:B:42:ASN:HD21	1:B:44:TYR:HB3	1.82	0.44
1:A:103:HIS:HD2	4:A:354:HOH:O	1.99	0.44
1:A:162:SER:HA	1:A:189:VAL:O	2.17	0.44
1:A:245:ILE:CD1	1:A:251:ILE:HD11	2.47	0.44
1:A:273:ILE:HD13	1:A:273:ILE:C	2.43	0.44
1:B:163:PHE:CE1	1:B:178:ILE:HD12	2.53	0.44
1:B:136:ASN:C	1:B:136:ASN:ND2	2.76	0.44
1:B:211:ALA:C	1:B:213:GLN:H	2.25	0.43
1:B:281:ARG:O	1:B:284:GLN:HG2	2.17	0.43
1:A:198:TYR:CG	1:A:199:ALA:N	2.85	0.43
1:A:281:ARG:NH2	1:A:284:GLN:OE1	2.52	0.43
1:B:153:LEU:HD23	1:B:154:THR:H	1.84	0.43
1:A:234:LEU:HD23	1:A:234:LEU:C	2.44	0.43
1:B:36:ARG:HG2	1:B:36:ARG:HH21	1.83	0.43
1:B:304:VAL:HG12	1:B:305:PRO:HD2	1.99	0.43
1:A:70:ILE:CD1	1:A:92:PHE:HB2	2.46	0.43
1:B:115:GLU:OE2	1:B:155:VAL:HG22	2.18	0.43
1:A:19:ILE:HD12	1:A:45:VAL:CG1	2.49	0.43
1:A:169:LEU:HB2	1:A:196:ILE:CD1	2.49	0.43
1:A:230:ARG:HA	1:A:230:ARG:HD3	1.71	0.43
1:B:248:ALA:O	1:B:251:ILE:HD13	2.18	0.43
1:A:169:LEU:HB2	1:A:196:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:HE2	4:A:377:HOH:O	2.18	0.43
1:A:111:ARG:NH2	1:A:111:ARG:HB2	2.34	0.43
1:B:127:VAL:O	1:B:131:MET:HG2	2.18	0.42
1:B:306:LYS:HA	1:B:309:ARG:HG3	2.01	0.42
1:A:117:ILE:CD1	1:A:153:LEU:HD11	2.44	0.42
1:B:135:SER:O	1:B:137:PRO:HD3	2.19	0.42
1:A:98:LEU:HA	1:A:98:LEU:HD12	1.77	0.42
1:A:154:THR:HB	4:A:480:HOH:O	2.19	0.42
1:A:247:ASP:OD1	1:A:249:LYS:HB2	2.19	0.42
1:B:304:VAL:HG13	1:B:305:PRO:HD2	2.02	0.42
1:B:245:ILE:HB	1:B:250:ASP:HB2	2.01	0.42
1:B:234:LEU:C	1:B:234:LEU:HD23	2.44	0.42
1:B:251:ILE:N	1:B:251:ILE:CD1	2.83	0.42
1:B:203:ARG:NH2	1:B:203:ARG:HG3	2.34	0.42
1:A:2:GLN:HG2	1:A:4:LEU:HD13	2.02	0.42
1:A:221:GLY:O	1:A:244:LEU:HD22	2.19	0.42
1:B:42:ASN:HD22	1:B:45:VAL:HG23	1.83	0.42
1:B:6:ALA:HB2	1:B:210:LEU:HD22	2.01	0.41
1:A:57:ILE:HD12	1:A:57:ILE:C	2.44	0.41
1:A:153:LEU:HD23	1:A:154:THR:H	1.84	0.41
1:B:36:ARG:HG2	1:B:36:ARG:NH2	2.34	0.41
1:A:42:ASN:HA	1:A:222:SER:OG	2.20	0.41
1:B:203:ARG:HG3	1:B:203:ARG:HH21	1.86	0.41
1:B:117:ILE:CD1	1:B:153:LEU:HD11	2.47	0.41
1:B:219:VAL:O	1:B:245:ILE:HD13	2.21	0.41
1:A:153:LEU:HD22	1:A:155:VAL:HG13	2.03	0.41
1:B:300:ILE:HG12	4:B:529:HOH:O	2.19	0.41
1:A:251:ILE:HD12	1:A:251:ILE:H	1.86	0.40
1:B:42:ASN:O	1:B:46:VAL:HG23	2.21	0.40
1:A:136:ASN:HD22	1:A:137:PRO:CD	2.35	0.40
1:B:60:ILE:HD12	1:B:83:GLU:HB3	2.02	0.40
1:B:196:ILE:HD12	1:B:196:ILE:H	1.85	0.40
1:B:5:LEU:HD12	1:B:264:VAL:CG1	2.52	0.40
1:B:230:ARG:HH21	1:B:233:GLU:CD	2.28	0.40
1:A:24:ASN:O	1:A:28:ILE:HG12	2.22	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%)	297 (97%)	10 (3%)	0	100	100
1	B	308/326 (94%)	301 (98%)	7 (2%)	0	100	100
All	All	615/652 (94%)	598 (97%)	17 (3%)	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%)	247 (96%)	10 (4%)	28	28
1	B	258/273 (94%)	247 (96%)	11 (4%)	26	25
All	All	515/546 (94%)	494 (96%)	21 (4%)	27	26

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

Mol	Chain	Res	Type
1	A	4	LEU
1	A	69	LEU
1	A	98	LEU
1	A	118	LEU
1	A	153	LEU
1	A	230	ARG
1	A	231	LEU
1	A	237	ARG

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Mol	Chain	Res	Type
1	A	244	LEU
1	A	273	ILE
1	B	4	LEU
1	B	69	LEU
1	B	98	LEU
1	B	112	ARG
1	B	148	ASP
1	B	161	LEU
1	B	231	LEU
1	B	244	LEU
1	B	245	ILE
1	B	281	ARG
1	B	285	LEU

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

Mol	Chain	Res	Type
1	A	42	ASN
1	A	78	GLN
1	A	103	HIS
1	A	121	HIS
1	A	133	GLN
1	A	136	ASN
1	A	213	GLN
1	A	236	GLN
1	A	252	GLN
1	A	277	ASN
1	A	283	GLN
1	B	2	GLN
1	B	7	ASN
1	B	37	HIS
1	B	42	ASN
1	B	78	GLN
1	B	103	HIS
1	B	133	GLN
1	B	136	ASN
1	B	213	GLN
1	B	229	ASN
1	B	236	GLN
1	B	252	GLN
1	B	276	GLN
1	B	277	ASN

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Mol	Chain	Res	Type
1	B	283	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	IPE	A	998	-	12,13,13	2.54	4 (33%)	16,19,19	1.28	3 (18%)
3	F3S	A	997	1	0,9,9	-	-	-		
2	IPE	B	998	-	12,13,13	2.52	3 (25%)	16,19,19	1.24	3 (18%)
3	F3S	B	997	1	0,9,9	-	-	-		

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	IPE	A	998	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	F3S	A	997	1	-	-	0/3/3/3
2	IPE	B	998	-	-	5/13/13/13	-
3	F3S	B	997	1	-	-	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	IPE	C4-C3	6.66	1.52	1.33
2	A	998	IPE	C4-C3	6.43	1.51	1.33
2	A	998	IPE	C5-C3	-3.89	1.33	1.48
2	B	998	IPE	C5-C3	-3.85	1.34	1.48
2	A	998	IPE	PB-O2B	2.91	1.59	1.50
2	B	998	IPE	PB-O2B	2.46	1.58	1.50
2	A	998	IPE	PA-O3A	2.01	1.61	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	IPE	O1B-PB-O3A	3.26	115.57	104.64
2	B	998	IPE	O1B-PB-O3A	3.25	115.55	104.64
2	A	998	IPE	C2-C3-C4	-2.39	116.77	123.13
2	B	998	IPE	C2-C3-C4	-2.36	116.85	123.13
2	A	998	IPE	C5-C3-C2	2.05	120.60	114.96
2	B	998	IPE	C5-C3-C2	2.03	120.53	114.96

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	998	IPE	C2-C1-O1-PA
2	A	998	IPE	C1-C2-C3-C5
2	A	998	IPE	PA-O3A-PB-O1B
2	B	998	IPE	C1-C2-C3-C5
2	B	998	IPE	PA-O3A-PB-O1B
2	B	998	IPE	C2-C1-O1-PA
2	A	998	IPE	C1-C2-C3-C4
2	B	998	IPE	C1-C2-C3-C4
2	A	998	IPE	PA-O3A-PB-O2B
2	A	998	IPE	PA-O3A-PB-O3B
2	B	998	IPE	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	997	F3S	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	309/326 (94%)	0.11	5 (1%) 70 70	6, 19, 33, 45	0
1	B	310/326 (95%)	0.01	4 (1%) 75 74	7, 18, 32, 46	0
All	All	619/652 (94%)	0.06	9 (1%) 72 71	6, 18, 33, 46	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	LYS	3.0
1	B	88	ASP	2.8
1	B	310	VAL	2.7
1	B	112	ARG	2.4
1	A	289	GLU	2.2
1	A	112	ARG	2.2
1	A	111	ARG	2.1
1	A	309	ARG	2.1
1	B	309	ARG	2.1

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 oligosaccharides 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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	F3S	A	997	7/7	0.91	0.09	10,12,15,18	0
3	F3S	B	997	7/7	0.93	0.07	11,13,15,16	0
2	IPE	A	998	14/14	0.96	0.08	9,13,22,24	0
2	IPE	B	998	14/14	0.96	0.08	7,10,16,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.