



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:32 AM GMT

PDB ID : 3KRC
Title : Mint heterotetrameric geranyl pyrophosphate synthase in complex with IPP
Authors : Chang, T.-H.; Hsieh, F.-L.; Ko, T.-P.; Wang, A.H.-J.
Deposited on : 2009-11-18
Resolution : 2.30 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>

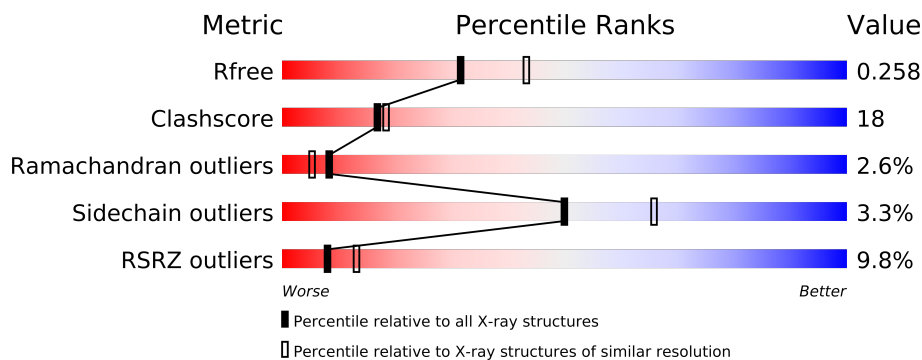
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	295	
1	D	295	
2	B	274	
2	C	274	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8913 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 Geranyl diphosphate synthase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2120	1338	372	392	18			
1	D	277	Total	C	N	O	S	0	0	0
			2102	1326	368	390	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9SBR3
D	1	MET	-	EXPRESSION TAG	UNP Q9SBR3

- Molecule 2 is a protein called Geranyl diphosphate synthase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			1954	1233	339	368	14			
2	C	271	Total	C	N	O	S	0	0	0
			2056	1297	361	384	14			

There are 18 discrepancies between the modelled and reference sequences:

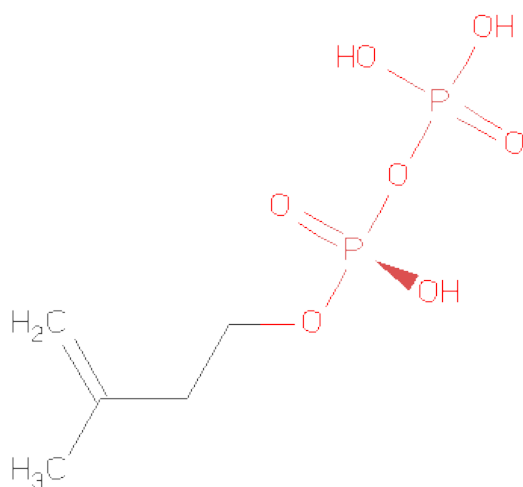
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP Q9SBR4
B	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	273	HIS	-	EXPRESSION TAG	UNP Q9SBR4
B	274	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	1	MET	-	EXPRESSION TAG	UNP Q9SBR4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	268	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	269	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	270	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	271	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	272	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	273	HIS	-	EXPRESSION TAG	UNP Q9SBR4
C	274	HIS	-	EXPRESSION TAG	UNP Q9SBR4

- 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		
3	D	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



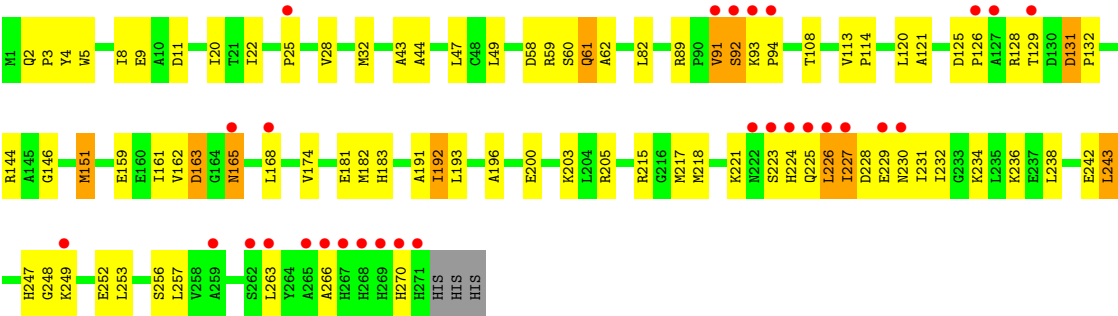
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	144	Total	O	0	0
			144	144		
5	C	153	Total	O	0	0
			153	153		
5	D	189	Total	O	0	0
			189	189		

● Molecule 2: Geranyl diphosphate synthase small subunit

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.12Å 108.97Å 182.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.76 – 2.28	Depositor EDS
% Data completeness (in resolution range)	88.2 (30.00-2.30) 87.1 (29.76-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.257 0.193 , 0.258	Depositor DCC
R_{free} test set	2163 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43739 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8913	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: EDO, 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	0.99	0/2155	0.93	1/2903 (0.0%)
1	D	0.88	0/2137	0.89	2/2881 (0.1%)
2	B	0.87	0/1993	0.85	0/2695
2	C	0.89	0/2102	0.85	1/2845 (0.0%)
All	All	0.91	0/8387	0.88	4/11324 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	MET	CG-SD-CE	5.58	109.13	100.20
2	C	144	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	43	GLY	N-CA-C	-5.35	99.74	113.10
1	D	61	ASP	CB-CG-OD2	-5.08	113.73	118.30

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	2120	0	2146	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2102	0	2120	99	0
2	B	1954	0	1948	75	1
2	C	2056	0	2031	71	0
3	A	14	0	9	2	0
3	D	14	0	9	1	0
4	C	4	0	6	0	0
5	A	163	0	0	6	1
5	B	144	0	0	4	0
5	C	153	0	0	5	0
5	D	189	0	0	8	0
All	All	8913	0	8269	294	1

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 18.

All (294) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:168:LEU:HD22	2:C:231:ILE:HD12	1.43	0.98
2:B:249:LYS:HG3	2:B:253:LEU:HB3	1.43	0.96
1:A:17:LYS:HE2	5:A:355:HOH:O	1.64	0.96
1:D:177:HIS:CB	1:D:218:GLN:HG2	1.97	0.94
2:B:249:LYS:HZ3	2:B:253:LEU:HA	1.32	0.94
2:B:54:LEU:HD13	2:B:253:LEU:HD21	1.46	0.94
1:D:177:HIS:HB3	1:D:218:GLN:HG2	1.54	0.89
2:B:54:LEU:CD1	2:B:253:LEU:HD21	2.02	0.87
1:D:168:VAL:HG21	1:D:246:THR:CG2	2.05	0.87
2:B:2:GLN:H	2:B:3:PRO:HD2	1.39	0.86
2:C:2:GLN:HB3	2:C:3:PRO:HD2	1.57	0.85
1:D:254:VAL:HA	1:D:257:SER:HB3	1.60	0.82
1:D:181:THR:HB	1:D:218:GLN:OE1	1.80	0.80
1:D:94:ARG:O	1:D:95:ARG:HB2	1.81	0.80
1:D:168:VAL:HG21	1:D:246:THR:HG23	1.62	0.78
2:B:93:LYS:HB3	2:B:94:PRO:HD3	1.64	0.78
2:C:58:ASP:O	2:C:61:GLN:HG2	1.83	0.77
1:A:276:HIS:HD2	1:A:279:ARG:NH2	1.82	0.76
2:C:168:LEU:HD22	2:C:231:ILE:CD1	2.16	0.76
2:B:255:SER:O	2:B:258:VAL:HG22	1.87	0.75
2:B:218:MET:HG2	2:B:221:LYS:NZ	2.03	0.73
1:A:228:LYS:HD2	1:A:228:LYS:H	1.54	0.72
1:D:263:ARG:NH1	5:D:544:HOH:O	2.10	0.70
2:C:125:ASP:HB3	2:C:128:ARG:HG3	1.74	0.70
1:A:165:MET:HG2	1:A:166:ALA:N	2.07	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:163:ASP:HA	2:B:224:HIS:HE1	1.57	0.69
1:D:149:SER:O	1:D:154:ALA:HB2	1.92	0.69
1:D:176:ILE:O	1:D:180:LYS:HG2	1.92	0.69
2:B:214:LEU:HD11	2:B:232:ILE:HG23	1.73	0.69
2:B:226:LEU:O	2:B:228:ASP:N	2.23	0.69
1:D:255:GLU:O	1:D:256:LYS:HG3	1.93	0.68
2:C:61:GLN:NE2	2:C:128:ARG:HH22	1.91	0.68
2:B:221:LYS:HE2	2:B:227:ILE:HG23	1.75	0.68
1:A:48:PRO:HG3	1:A:73:GLU:HB2	1.75	0.68
1:D:177:HIS:CG	1:D:218:GLN:HG2	2.27	0.68
1:A:186:GLN:NE2	1:A:211:ASN:OD1	2.26	0.68
1:A:165:MET:HG2	1:A:166:ALA:H	1.59	0.67
2:B:249:LYS:O	2:B:253:LEU:N	2.27	0.67
1:D:168:VAL:HG21	1:D:246:THR:HG21	1.75	0.67
2:B:218:MET:HG2	2:B:221:LYS:HZ2	1.59	0.67
2:C:217:MET:CE	2:C:231:ILE:HG21	2.25	0.66
5:C:299:HOH:O	1:D:161:CYS:SG	2.53	0.66
2:C:89:ARG:NH1	5:C:355:HOH:O	2.29	0.66
2:C:230:ASN:O	2:C:234:LYS:HG3	1.96	0.65
2:C:165:ASN:ND2	2:C:165:ASN:O	2.29	0.65
2:C:248:GLY:HA3	5:C:648:HOH:O	1.96	0.65
2:B:163:ASP:HA	2:B:224:HIS:CE1	2.31	0.65
1:A:262:ASP:OD2	5:A:523:HOH:O	2.14	0.65
2:B:249:LYS:HZ3	2:B:253:LEU:CA	2.08	0.65
1:A:75:ILE:HG21	1:A:147:ILE:HG21	1.77	0.65
2:C:91:VAL:HG11	5:C:389:HOH:O	1.96	0.65
2:C:4:TYR:CZ	2:C:8:ILE:HD11	2.32	0.65
2:C:266:ALA:O	2:C:270:HIS:ND1	2.30	0.64
2:B:253:LEU:HG	2:B:254:MET:HE2	1.78	0.64
2:B:167:SER:OG	1:D:33:GLU:OE2	2.14	0.63
2:B:233:GLY:O	2:B:236:LYS:HG2	1.99	0.63
1:D:93:LEU:HD23	1:D:98:PRO:HA	1.81	0.63
1:D:149:SER:C	1:D:154:ALA:HB2	2.21	0.61
2:B:250:ASN:C	2:B:252:GLU:H	2.02	0.61
1:A:259:GLU:O	1:A:263:ARG:HG3	2.00	0.61
2:C:5:TRP:CH2	2:C:257:LEU:HD22	2.36	0.61
2:C:215:ARG:HH11	2:C:215:ARG:HG2	1.66	0.61
2:B:171:ILE:HG22	2:B:217:MET:CE	2.31	0.60
1:A:82:HIS:ND1	2:B:110:ASP:OD2	2.31	0.60
1:A:76:HIS:HE1	3:A:902:IPE:H21	1.67	0.60
2:C:43:ALA:O	2:C:47:LEU:HB2	2.02	0.60
1:A:245:LYS:N	1:A:245:LYS:HD3	2.17	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:221:LYS:HE2	2:C:227:ILE:HG21	1.84	0.60
2:C:168:LEU:HD13	2:C:231:ILE:HD11	1.84	0.60
2:B:227:ILE:HG22	2:B:232:ILE:HD11	1.82	0.60
2:B:2:GLN:H	2:B:3:PRO:CD	2.14	0.59
2:B:237:GLU:O	2:B:241:GLU:HB2	2.02	0.59
1:D:173:LEU:HD11	1:D:247:THR:HA	1.82	0.59
1:D:94:ARG:O	1:D:95:ARG:CB	2.47	0.59
2:C:218:MET:HA	2:C:221:LYS:HD2	1.82	0.59
2:B:14:ARG:NH1	2:B:14:ARG:HB2	2.17	0.59
1:A:79:SER:O	1:A:83:ASP:HB2	2.02	0.59
2:B:168:LEU:HD11	2:B:226:LEU:HG	1.85	0.58
2:B:93:LYS:CB	2:B:94:PRO:HD3	2.31	0.58
1:D:265:ASN:O	1:D:269:GLN:HG3	2.04	0.58
1:D:199:LYS:NZ	5:D:517:HOH:O	2.29	0.58
2:B:54:LEU:HD11	2:B:250:ASN:HA	1.86	0.58
3:A:902:IPE:H53	5:A:372:HOH:O	2.03	0.58
1:D:256:LYS:HA	1:D:259:GLU:HB3	1.86	0.57
2:B:60:SER:HB2	5:B:502:HOH:O	2.04	0.57
1:A:227:THR:HB	1:A:228:LYS:HD2	1.87	0.57
1:D:97:LYS:HB2	1:D:98:PRO:HD2	1.87	0.57
1:A:138:ARG:HD3	5:A:488:HOH:O	2.03	0.57
2:B:249:LYS:HD2	2:B:252:GLU:HB3	1.87	0.57
1:A:276:HIS:CD2	1:A:279:ARG:NH2	2.69	0.57
1:A:159:ASP:OD1	1:A:176:ILE:HD13	2.05	0.57
2:B:222:ASN:HA	5:B:560:HOH:O	2.04	0.56
2:B:249:LYS:O	2:B:253:LEU:HD23	2.05	0.56
2:C:61:GLN:HE21	2:C:128:ARG:HH22	1.51	0.56
2:B:35:LEU:HD12	2:B:108:THR:HG21	1.86	0.56
1:D:207:ARG:O	1:D:210:ALA:HB3	2.05	0.56
1:D:252:ILE:HD12	1:D:256:LYS:HB3	1.88	0.56
1:A:171:ASP:HB3	5:A:396:HOH:O	2.05	0.56
2:C:225:GLN:O	2:C:226:LEU:HB2	2.05	0.56
1:D:94:ARG:HG2	1:D:95:ARG:HG3	1.88	0.56
1:D:75:ILE:HG21	1:D:147:ILE:HG21	1.88	0.55
1:D:180:LYS:O	1:D:181:THR:CB	2.55	0.55
2:C:125:ASP:HB3	2:C:128:ARG:CG	2.36	0.55
1:D:181:THR:HA	5:D:630:HOH:O	2.07	0.55
2:C:228:ASP:C	2:C:230:ASN:H	2.11	0.54
2:B:71:LEU:HD22	2:B:112:ILE:HG23	1.89	0.54
1:D:168:VAL:HG12	1:D:172:HIS:CD2	2.42	0.54
2:C:82:LEU:O	2:C:89:ARG:NH2	2.41	0.54
1:D:30:LYS:HE2	1:D:104:PHE:HD2	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:LYS:HD2	1:A:228:LYS:N	2.21	0.54
2:B:164:GLY:O	2:B:165:ASN:HB2	2.06	0.54
1:D:76:HIS:HE1	3:D:901:IPE:H11	1.72	0.53
1:D:170:LEU:O	1:D:174:GLU:HB2	2.09	0.53
1:D:199:LYS:HG2	1:D:202:GLU:OE1	2.09	0.53
1:D:87:CYS:SG	5:D:338:HOH:O	2.58	0.53
2:B:188:ALA:O	2:B:192:ILE:HG13	2.08	0.53
2:C:162:VAL:O	2:C:165:ASN:HB3	2.09	0.53
1:A:95:ARG:O	1:A:97:LYS:HG3	2.09	0.53
1:D:247:THR:OG1	1:D:249:PRO:HD2	2.09	0.53
1:D:168:VAL:O	1:D:168:VAL:HG23	2.09	0.52
2:C:217:MET:HE2	2:C:231:ILE:HG21	1.91	0.52
2:C:3:PRO:HG2	2:C:4:TYR:H	1.73	0.52
1:D:186:GLN:NE2	1:D:211:ASN:ND2	2.57	0.52
1:D:177:HIS:CA	1:D:218:GLN:HG2	2.40	0.52
2:B:14:ARG:HH11	2:B:14:ARG:HB2	1.75	0.52
1:D:45:ARG:HB3	1:D:48:PRO:HG2	1.92	0.52
2:C:161:ILE:HD11	2:C:174:VAL:HG21	1.91	0.52
1:D:68:ALA:HA	1:D:124:VAL:HG22	1.91	0.52
1:A:276:HIS:CD2	1:A:279:ARG:HH21	2.28	0.51
2:C:9:GLU:HG2	5:C:276:HOH:O	2.10	0.51
2:B:249:LYS:O	2:B:252:GLU:N	2.43	0.51
1:D:152:LEU:C	1:D:152:LEU:HD23	2.31	0.51
1:A:166:ALA:O	1:A:168:VAL:N	2.32	0.51
2:C:91:VAL:O	2:C:92:SER:C	2.48	0.51
2:C:92:SER:O	2:C:93:LYS:C	2.49	0.51
2:B:249:LYS:CG	2:B:253:LEU:HB3	2.28	0.51
1:D:176:ILE:HG22	1:D:180:LYS:CD	2.40	0.51
1:A:159:ASP:OD1	1:A:176:ILE:HG21	2.09	0.51
2:C:231:ILE:O	2:C:234:LYS:HB2	2.10	0.51
1:D:168:VAL:HG12	1:D:172:HIS:HD2	1.74	0.51
1:D:168:VAL:HG11	1:D:246:THR:HG21	1.91	0.51
2:C:44:ALA:HB2	2:C:183:HIS:CD2	2.45	0.51
1:D:152:LEU:HA	1:D:179:HIS:O	2.11	0.51
2:C:162:VAL:HG12	2:C:163:ASP:OD2	2.11	0.50
1:D:253:GLY:O	1:D:255:GLU:N	2.44	0.50
2:B:213:THR:O	2:B:217:MET:HB2	2.11	0.50
2:C:253:LEU:O	2:C:256:SER:OG	2.30	0.50
2:C:5:TRP:CZ2	2:C:257:LEU:HB2	2.47	0.50
1:A:29:LEU:O	1:A:33:GLU:HB2	2.12	0.50
1:D:177:HIS:HB3	1:D:218:GLN:CG	2.35	0.49
1:D:186:GLN:CD	1:D:211:ASN:ND2	2.66	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:276:HIS:HD2	1:A:279:ARG:HH21	1.55	0.49
1:A:219:VAL:O	1:A:223:ILE:HG13	2.12	0.49
1:A:133:PRO:O	1:A:137:VAL:HG23	2.13	0.49
2:C:163:ASP:HA	2:C:224:HIS:CE1	2.48	0.49
1:D:176:ILE:HG22	1:D:180:LYS:HD2	1.94	0.49
2:B:103:ASN:O	2:B:107:LEU:HG	2.13	0.49
1:D:154:ALA:O	1:D:158:VAL:HG23	2.12	0.49
1:A:168:VAL:HG13	1:A:172:HIS:CD2	2.48	0.48
2:C:159:GLU:OE2	1:D:107:SER:OG	2.31	0.48
2:B:176:LYS:O	2:B:181:GLU:HG2	2.13	0.48
2:C:93:LYS:N	2:C:94:PRO:HD2	2.29	0.48
2:C:62:ALA:HA	2:C:193:LEU:HD13	1.95	0.48
2:C:181:GLU:HA	2:C:181:GLU:OE2	2.14	0.48
1:D:219:VAL:HG22	1:D:248:TYR:CD2	2.49	0.47
1:D:254:VAL:C	1:D:256:LYS:H	2.18	0.47
1:D:224:LEU:HD22	1:D:294:ASP:O	2.13	0.47
1:A:137:VAL:HA	1:A:140:LEU:HD12	1.97	0.47
1:A:256:LYS:HG2	5:A:401:HOH:O	2.14	0.47
2:B:249:LYS:C	2:B:253:LEU:HD23	2.35	0.47
2:B:171:ILE:HG22	2:B:217:MET:HE1	1.95	0.47
1:D:246:THR:N	5:D:601:HOH:O	2.48	0.47
2:C:191:ALA:O	2:C:192:ILE:C	2.52	0.47
2:C:215:ARG:NH1	2:C:215:ARG:HG2	2.29	0.47
1:D:156:GLN:NE2	5:D:344:HOH:O	2.48	0.46
2:C:3:PRO:HG2	2:C:4:TYR:N	2.30	0.46
1:D:157:VAL:HA	1:D:160:VAL:HG22	1.97	0.46
1:A:99:THR:OG1	1:A:102:MET:HG2	2.15	0.46
1:D:4:PHE:HB2	1:D:8:MET:CE	2.45	0.46
2:B:250:ASN:C	2:B:252:GLU:N	2.68	0.46
1:D:178:HIS:C	1:D:182:ALA:HB3	2.35	0.46
2:C:58:ASP:O	2:C:60:SER:N	2.48	0.46
1:D:176:ILE:CG2	1:D:180:LYS:HD2	2.45	0.46
1:D:71:ALA:O	1:D:75:ILE:HG12	2.15	0.46
1:D:41:ALA:HB3	1:D:95:ARG:HH11	1.81	0.46
1:D:23:VAL:O	1:D:36:ARG:HD2	2.16	0.46
1:A:47:ARG:HB2	1:A:48:PRO:HD3	1.97	0.46
1:A:158:VAL:HG12	1:A:176:ILE:HG12	1.98	0.45
2:C:32:MET:HA	2:C:108:THR:CG2	2.46	0.45
2:B:62:ALA:HA	2:B:193:LEU:HD13	1.98	0.45
1:A:201:GLU:O	1:A:205:LYS:HG2	2.16	0.45
1:D:290:ILE:HA	1:D:293:ARG:HD3	1.98	0.45
1:D:172:HIS:HB2	5:D:637:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2:GLN:N	2:B:3:PRO:HD2	2.19	0.45
1:A:95:ARG:HD2	1:A:95:ARG:N	2.32	0.45
1:D:45:ARG:O	1:D:48:PRO:HG2	2.17	0.45
1:D:9:LEU:HA	1:D:9:LEU:HD23	1.82	0.45
2:B:173:TYR:CE2	1:D:29:LEU:HD21	2.52	0.45
1:D:111:LEU:HA	1:D:111:LEU:HD23	1.78	0.45
1:D:170:LEU:HD23	1:D:251:LEU:HD12	1.98	0.45
1:A:66:MET:HB3	1:A:67:PRO:HD3	1.97	0.45
1:D:179:HIS:O	1:D:181:THR:N	2.43	0.45
1:A:177:HIS:CG	1:A:218:GLN:HG3	2.52	0.45
1:D:177:HIS:CG	1:D:218:GLN:CG	3.00	0.45
2:B:75:ALA:CB	2:B:113:VAL:HG23	2.47	0.45
2:B:87:GLY:N	5:B:646:HOH:O	2.31	0.45
1:D:173:LEU:HD21	1:D:248:TYR:N	2.32	0.44
1:D:248:TYR:N	1:D:249:PRO:CD	2.79	0.44
1:D:246:THR:HA	1:D:250:LYS:CD	2.48	0.44
1:D:162:SER:HB3	1:D:165:MET:HG3	1.99	0.44
1:D:26:LYS:NZ	5:D:326:HOH:O	2.30	0.44
2:C:232:ILE:O	2:C:236:LYS:HB2	2.17	0.44
2:B:249:LYS:NZ	2:B:253:LEU:CB	2.80	0.44
2:B:171:ILE:HG22	2:B:217:MET:HE3	1.99	0.44
2:C:221:LYS:HB2	2:C:227:ILE:HG21	1.98	0.44
1:D:249:PRO:O	1:D:253:GLY:HA2	2.18	0.44
2:B:214:LEU:O	2:B:217:MET:HB3	2.17	0.44
1:D:281:ALA:HB3	1:D:282:PRO:HD3	1.99	0.44
2:B:200:GLU:HB3	2:B:246:PHE:CZ	2.52	0.44
1:D:86:PRO:HA	1:D:90:ASN:HB2	1.99	0.44
1:D:173:LEU:HD21	1:D:247:THR:C	2.37	0.44
1:A:199:LYS:O	1:A:203:VAL:HG23	2.17	0.44
1:D:174:GLU:O	1:D:178:HIS:HB2	2.17	0.44
2:B:43:ALA:HB3	2:B:183:HIS:CE1	2.53	0.44
1:D:180:LYS:HG3	1:D:180:LYS:O	2.17	0.44
1:A:177:HIS:ND1	1:A:218:GLN:HG3	2.33	0.43
2:C:146:GLY:HA2	2:C:151:MET:HE2	1.99	0.43
2:C:113:VAL:HB	2:C:114:PRO:CD	2.48	0.43
1:D:246:THR:HA	1:D:250:LYS:HD2	2.00	0.43
2:B:246:PHE:O	2:B:247:HIS:O	2.35	0.43
1:A:222:ASP:HB3	1:A:249:PRO:HD3	2.01	0.43
1:D:181:THR:HG22	1:D:182:ALA:N	2.33	0.43
1:A:94:ARG:O	1:A:95:ARG:HB2	2.18	0.43
2:B:128:ARG:NH1	5:B:349:HOH:O	2.40	0.43
1:D:99:THR:OG1	1:D:102:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:226:LEU:O	2:C:228:ASP:N	2.52	0.43
2:C:217:MET:HE3	2:C:231:ILE:HG21	2.00	0.43
1:D:152:LEU:O	1:D:152:LEU:HD23	2.18	0.43
1:D:178:HIS:O	1:D:182:ALA:HB3	2.19	0.42
2:B:218:MET:HG2	2:B:221:LYS:CE	2.48	0.42
1:A:245:LYS:CD	1:A:245:LYS:N	2.79	0.42
2:C:243:LEU:HD23	2:C:243:LEU:HA	1.78	0.42
2:C:238:LEU:O	2:C:242:GLU:HG2	2.19	0.42
2:B:250:ASN:O	2:B:252:GLU:N	2.52	0.42
1:D:80:LEU:HD13	1:D:94:ARG:NH2	2.34	0.42
2:B:227:ILE:CG2	2:B:232:ILE:HD11	2.46	0.42
2:C:227:ILE:O	2:C:227:ILE:HG23	2.18	0.42
2:C:25:PRO:HG2	2:C:28:VAL:CG2	2.48	0.42
2:B:31:PRO:HB3	2:B:100:TYR:CE2	2.55	0.42
2:C:20:ILE:O	2:C:20:ILE:HG22	2.19	0.42
1:A:168:VAL:HB	1:A:246:THR:OG1	2.19	0.42
2:B:228:ASP:OD2	2:B:230:ASN:HB2	2.19	0.42
1:A:143:LEU:O	1:A:147:ILE:HG12	2.20	0.42
2:B:236:LYS:HG3	2:B:237:GLU:N	2.34	0.42
2:C:249:LYS:O	2:C:252:GLU:HB3	2.20	0.42
1:D:286:LEU:O	1:D:290:ILE:HG13	2.19	0.42
2:B:243:LEU:HB3	2:B:251:ALA:HA	1.99	0.42
2:C:228:ASP:C	2:C:230:ASN:N	2.72	0.42
2:C:8:ILE:O	2:C:11:ASP:HB2	2.20	0.42
1:D:94:ARG:HG2	1:D:94:ARG:O	2.17	0.42
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.85	0.42
1:D:180:LYS:O	1:D:181:THR:HB	2.19	0.42
1:D:179:HIS:C	1:D:181:THR:H	2.20	0.42
2:C:126:PRO:C	2:C:128:ARG:H	2.23	0.42
1:A:227:THR:HG21	1:A:228:LYS:NZ	2.35	0.42
1:A:157:VAL:O	1:A:160:VAL:HG22	2.20	0.41
2:B:200:GLU:HB3	2:B:246:PHE:CE2	2.55	0.41
2:B:214:LEU:CD2	2:B:218:MET:HE3	2.50	0.41
1:D:186:GLN:HA	1:D:210:ALA:HB1	2.02	0.41
1:A:86:PRO:HD3	1:A:101:HIS:CD2	2.55	0.41
2:B:221:LYS:CE	2:B:227:ILE:HG23	2.46	0.41
2:B:236:LYS:HE2	2:B:240:LEU:HD11	2.03	0.41
2:C:205:ARG:HG3	2:C:205:ARG:HH11	1.85	0.41
1:A:165:MET:CG	1:A:166:ALA:H	2.32	0.41
2:C:181:GLU:CA	2:C:181:GLU:OE2	2.68	0.41
1:D:151:GLY:O	1:D:179:HIS:HB3	2.20	0.41
2:B:192:ILE:HG12	2:B:201:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:252:GLU:C	2:B:254:MET:N	2.73	0.41
1:D:55:CYS:HA	1:D:192:GLY:O	2.21	0.41
1:A:276:HIS:HA	1:A:277:PRO:HD3	1.78	0.41
2:B:218:MET:HA	2:B:221:LYS:HG3	2.02	0.41
2:C:120:LEU:O	2:C:121:ALA:C	2.59	0.41
2:C:132:PRO:CG	1:D:134:GLU:HB3	2.51	0.41
2:C:4:TYR:CE2	2:C:8:ILE:HD11	2.55	0.41
2:C:93:LYS:HB3	2:C:94:PRO:HD3	2.03	0.41
1:D:147:ILE:O	1:D:153:VAL:HG23	2.20	0.41
2:C:131:ASP:CB	2:C:132:PRO:HD3	2.51	0.41
1:A:75:ILE:O	1:A:78:MET:HG3	2.21	0.40
1:A:151:GLY:O	1:A:152:LEU:C	2.60	0.40
2:B:69:ILE:CD1	2:B:186:GLY:HA2	2.51	0.40
2:C:8:ILE:HG23	2:C:49:LEU:HD12	2.03	0.40
2:B:43:ALA:HB3	2:B:183:HIS:HE1	1.86	0.40
2:C:200:GLU:O	2:C:203:LYS:N	2.51	0.40
2:B:24:PRO:HA	2:B:25:PRO:HA	1.81	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:246:PHE:O	5:A:509:HOH:O[3_545]	2.15	0.05

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	275/295 (93%)	261 (95%)	12 (4%)	2 (1%)	30	34
1	D	273/295 (92%)	251 (92%)	14 (5%)	8 (3%)	7	4
2	B	257/274 (94%)	239 (93%)	12 (5%)	6 (2%)	10	7
2	C	269/274 (98%)	242 (90%)	15 (6%)	12 (4%)	4	1
All	All	1074/1138 (94%)	993 (92%)	53 (5%)	28 (3%)	8	5

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	THR
2	B	165	ASN
2	B	227	ILE
2	B	247	HIS
2	C	226	LEU
2	C	227	ILE
2	C	247	HIS
1	D	162	SER
1	D	181	THR
1	D	254	VAL
1	D	256	LYS
1	A	167	GLU
2	C	22	ILE
2	C	59	ARG
2	C	92	SER
2	C	163	ASP
2	C	196	ALA
1	D	166	ALA
1	D	180	LYS
2	B	2	GLN
2	B	251	ALA
2	C	129	THR
2	C	229	GLU
1	D	95	ARG
2	B	221	LYS
1	D	253	GLY
2	C	192	ILE
2	C	91	VAL

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	222/234 (95%)	214 (96%)	8 (4%)	47	61
1	D	220/234 (94%)	215 (98%)	5 (2%)	63	80
2	B	201/214 (94%)	194 (96%)	7 (4%)	48	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	211/214 (99%)	203 (96%)	8 (4%)	44	59
All	All	854/896 (95%)	826 (97%)	28 (3%)	50	66

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	89	ASP
1	A	95	ARG
1	A	201	GLU
1	A	221	ASP
1	A	228	LYS
1	A	245	LYS
1	A	270	GLU
2	B	2	GLN
2	B	42	THR
2	B	73	HIS
2	B	211	GLN
2	B	220	MET
2	B	246	PHE
2	B	253	LEU
2	C	61	GLN
2	C	131	ASP
2	C	151	MET
2	C	165	ASN
2	C	182	MET
2	C	223	SER
2	C	243	LEU
2	C	263	LEU
1	D	118	SER
1	D	134	GLU
1	D	181	THR
1	D	262	ASP
1	D	294	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	90	ASN
1	A	156	GLN

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Mol	Chain	Res	Type
1	A	218	GLN
1	A	276	HIS
2	B	81	HIS
2	B	183	HIS
2	B	202	GLN
2	B	206	ASN
2	B	211	GLN
2	C	81	HIS
2	C	165	ASN
2	C	230	ASN
2	C	250	ASN
1	D	172	HIS
1	D	178	HIS
1	D	186	GLN
1	D	211	ASN

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 ⓘ

3 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	IPE	A	902	-	13,13,13	2.57	4 (30%)	19,19,19	2.05	7 (36%)
4	EDO	C	903	-	3,3,3	1.26	0	2,2,2	0.19	0
3	IPE	D	901	-	13,13,13	2.75	2 (15%)	19,19,19	1.97	8 (42%)

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	IPE	A	902	-	-	0/13/13/13	0/0/0/0
4	EDO	C	903	-	-	0/1/1/1	0/0/0/0
3	IPE	D	901	-	-	0/13/13/13	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	IPE	C4-C3	7.31	1.57	1.33
3	A	902	IPE	C4-C3	6.53	1.55	1.33
3	D	901	IPE	C2-C3	-6.21	1.37	1.51
3	A	902	IPE	C2-C3	-4.69	1.40	1.51
3	A	902	IPE	PA-O1A	2.36	1.60	1.51
3	A	902	IPE	PA-O3A	-2.15	1.56	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	IPE	O3A-PA-O1	4.61	124.04	103.41
3	D	901	IPE	O3A-PA-O1	4.30	122.66	103.41
3	A	902	IPE	C1-C2-C3	3.48	128.87	111.80
3	D	901	IPE	C1-C2-C3	3.03	126.67	111.80
3	D	901	IPE	O1B-PB-O3A	2.79	118.38	105.14
3	A	902	IPE	O1B-PB-O3A	2.75	118.17	105.14
3	A	902	IPE	PA-O3A-PB	-2.65	123.91	131.68
3	D	901	IPE	O3B-PB-O1B	-2.61	97.43	107.61
3	A	902	IPE	O3B-PB-O1B	-2.44	98.12	107.61
3	D	901	IPE	PA-O3A-PB	-2.20	125.22	131.68
3	D	901	IPE	O3B-PB-O3A	2.20	115.56	105.14
3	D	901	IPE	O1-C1-C2	2.16	118.77	108.62
3	D	901	IPE	O3B-PB-O2B	-2.16	103.37	110.44
3	A	902	IPE	O3A-PA-O1A	-2.12	96.08	111.28
3	A	902	IPE	O1-C1-C2	2.10	118.46	108.62

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	279/295 (94%)	0.02	16 (5%) 23 32	27, 41, 77, 108	0
1	D	277/295 (93%)	0.61	35 (12%) 4 7	27, 44, 120, 130	0
2	B	259/274 (94%)	0.31	27 (10%) 7 11	30, 47, 120, 136	0
2	C	271/274 (98%)	0.39	29 (10%) 6 10	27, 47, 102, 119	0
All	All	1086/1138 (95%)	0.33	107 (9%) 8 13	27, 44, 113, 136	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	166	ALA	12.2
1	D	165	MET	9.0
1	D	167	GLU	8.2
1	D	251	LEU	8.1
1	D	254	VAL	8.0
1	D	252	ILE	7.6
1	D	168	VAL	6.8
1	A	165	MET	6.5
1	D	172	HIS	6.3
1	D	163	GLU	6.3
2	B	258	VAL	6.0
2	C	263	LEU	5.9
1	D	173	LEU	5.8
1	D	164	GLY	5.7
1	D	256	LYS	5.6
1	D	170	LEU	5.5
1	D	169	GLY	5.5
2	C	127	ALA	5.3
1	A	164	GLY	5.2
2	C	262	SER	5.2
2	C	265	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
2	C	225	GLN	5.0
2	C	270	HIS	4.9
1	D	161	CYS	4.9
1	A	166	ALA	4.8
2	C	269	HIS	4.8
2	C	271	HIS	4.8
1	D	174	GLU	4.8
1	A	226	VAL	4.7
1	D	250	LYS	4.6
2	C	268	HIS	4.6
2	B	248	GLY	4.6
2	B	93	LYS	4.4
1	D	255	GLU	4.4
2	C	126	PRO	4.4
1	D	246	THR	4.3
1	D	162	SER	4.3
1	D	175	PHE	4.2
2	C	267	HIS	4.1
2	B	225	GLN	4.1
2	B	249	LYS	3.9
2	C	93	LYS	3.8
2	B	250	ASN	3.7
1	D	171	ASP	3.7
1	D	257	SER	3.6
2	C	224	HIS	3.6
2	B	231	ILE	3.5
1	A	168	VAL	3.5
1	D	178	HIS	3.5
2	B	247	HIS	3.4
2	C	129	THR	3.3
2	B	226	LEU	3.3
2	B	251	ALA	3.3
2	B	245	GLY	3.3
2	C	227	ILE	3.2
2	C	226	LEU	3.1
1	A	161	CYS	3.1
2	B	257	LEU	3.1
1	A	167	GLU	3.1
2	B	243	LEU	3.0
1	A	295	ASN	3.0
2	B	246	PHE	3.0
1	A	163	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	222	ASN	3.0
2	B	94	PRO	2.9
2	B	1	MET	2.9
2	C	266	ALA	2.9
2	C	249	LYS	2.9
2	B	222	ASN	2.9
1	A	228	LYS	2.9
1	D	157	VAL	2.9
1	D	160	VAL	2.8
1	A	117	LEU	2.6
2	C	165	ASN	2.6
2	C	91	VAL	2.6
2	B	152	ILE	2.6
1	A	294	ASP	2.5
1	A	91	ASP	2.5
1	D	247	THR	2.5
1	A	162	SER	2.5
1	D	184	LEU	2.4
2	C	230	ASN	2.3
1	D	226	VAL	2.3
1	D	79	SER	2.3
2	B	239	ALA	2.3
1	D	249	PRO	2.3
2	C	259	ALA	2.3
1	D	130	GLY	2.2
1	A	110	VAL	2.2
2	C	223	SER	2.2
2	B	236	LYS	2.2
1	A	246	THR	2.2
1	D	259	GLU	2.2
1	D	92	ASP	2.2
2	B	240	LEU	2.2
2	B	22	ILE	2.1
2	B	2	GLN	2.1
2	B	223	SER	2.1
2	B	254	MET	2.1
2	C	92	SER	2.1
2	B	259	ALA	2.1
2	B	24	PRO	2.1
2	C	229	GLU	2.1
2	C	25	PRO	2.1
2	C	168	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	94	PRO	2.0
1	D	187	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, 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
4	EDO	C	903	4/4	0.17	1.74	30,30,32,32	0
3	IPE	A	902	14/14	0.15	0.34	90,92,94,94	0
3	IPE	D	901	14/14	0.16	-0.21	55,60,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.