



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:32 AM GMT

PDB ID : 2XH1
Title : CRYSTAL STRUCTURE OF HUMAN KAT II-INHIBITOR COMPLEX
Authors : Rossi, F.; Casazza, V.; Garavaglia, S.; Sathyasaikumar, K.V.; Schwarcz, R.;
Kojima, S.I.; Okuwaki, K.; Ono, S.I.; Kajii, Y.; Rizzi, M.
Deposited on : 2010-06-08
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

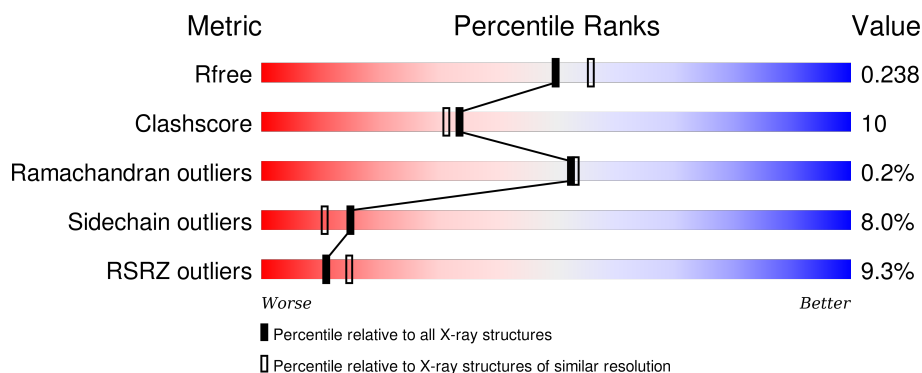
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	425	
1	B	425	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6972 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.

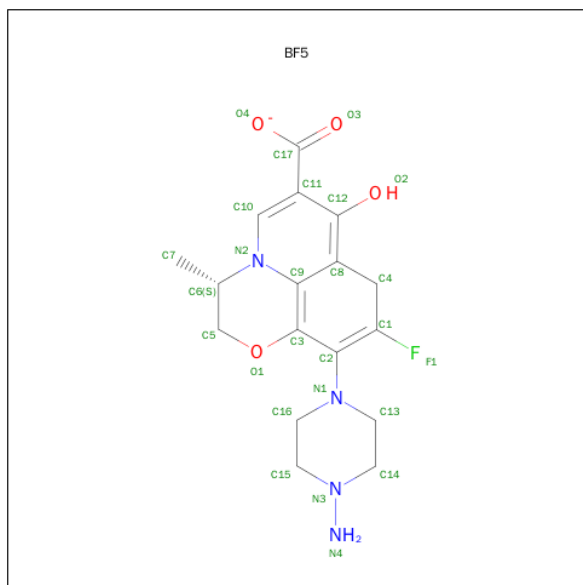
- Molecule 1 is a protein called KYNURENINE/ α -AMINOADIPATE AMINOTRANSFERASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3233	2079	539	599	16			
1	B	412	Total	C	N	O	S	0	0	0
			3234	2079	539	600	16			

There are 2 discrepancies between the modelled and reference sequences:

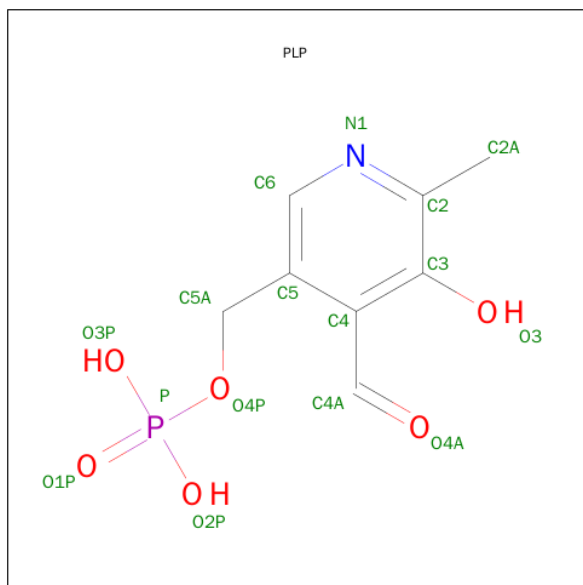
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	MET	ENGINEERED MUTATION	UNP Q8N5Z0
B	-1	GLU	MET	ENGINEERED MUTATION	UNP Q8N5Z0

- Molecule 2 is (3S)-10-(4-AMINOPIPERAZIN-1-YL)-9-FLUORO-7-HYDROXY-3-METHYL-2,3-DIHYDRO-8H-[1,4]OXAZINO[2,3,4-IJ]QUINOLINE-6-CARBOXYLATE (three-letter code: BF5) (formula: C₁₇H₁₉FN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			26	17	1	4	4		
2	B	1	Total	C	F	N	O	0	0
			26	17	1	4	4		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total	0	0
			1 I		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

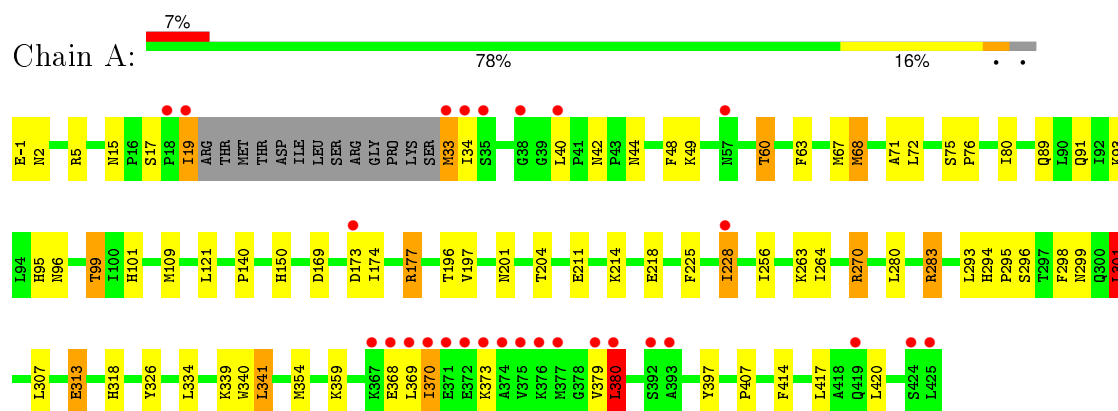
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	241	Total	O	0	0
			241	241		
6	B	175	Total	O	0	0
			175	175		

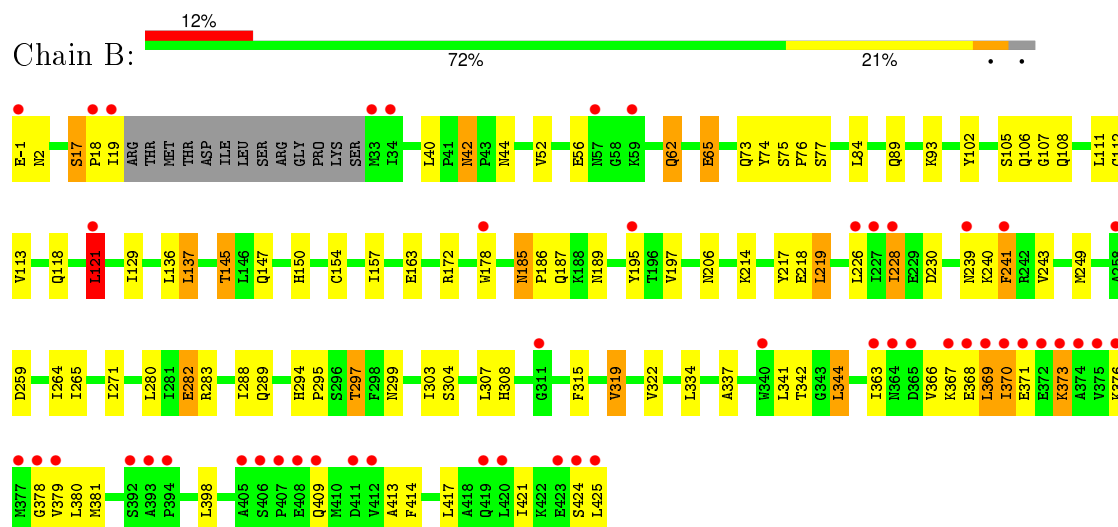
3 Residue-property plots [i](#)

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: KYNURENINE/ALPHA-AMINOADIPATE AMINOTRANSFERASE, MITOCHONDRIAL



• Molecule 1: KYNURENINE/ALPHA-AMINOADIPATE AMINOTRANSFERASE, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.32Å 152.86Å 60.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.04 – 2.10 30.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.04-2.10) 99.9 (30.73-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.241 0.191 , 0.238	Depositor DCC
R_{free} test set	1111 reflections (2.09%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 54286 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6972	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, IOD, BF5, PLP

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	0.91	1/3313 (0.0%)	0.84	4/4498 (0.1%)
1	B	0.84	2/3314 (0.1%)	0.87	7/4498 (0.2%)
All	All	0.87	3/6627 (0.0%)	0.85	11/8996 (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
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	GLU	CD-OE1	6.42	1.32	1.25
1	B	107	GLY	N-CA	5.76	1.54	1.46
1	A	225	PHE	CE1-CZ	5.43	1.47	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH1	10.15	125.37	120.30
1	B	106	GLN	C-N-CA	-9.45	102.46	122.30
1	B	283	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	B	137	LEU	CA-CB-CG	7.89	133.46	115.30
1	A	380	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	270	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	169	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	A	301	LEU	CB-CG-CD1	5.35	120.10	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	121	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	106	GLN	O-C-N	-5.09	114.55	123.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	GLU	Peptide

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	3233	0	3241	67	1
1	B	3234	0	3241	71	0
2	A	26	0	17	4	0
2	B	26	0	17	1	0
3	A	15	0	6	0	0
3	B	15	0	7	0	0
4	A	1	0	0	0	0
5	B	6	0	8	0	0
6	A	241	0	0	14	0
6	B	175	0	0	8	0
All	All	6972	0	6537	133	1

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 10.

All (133) 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:89:GLN:HG3	1:B:93:LYS:HE2	1.42	0.99
1:B:112:CYS:HB2	6:B:2076:HOH:O	1.66	0.94
1:A:99:THR:HG21	6:A:2073:HOH:O	1.71	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:CYS:SG	6:B:2076:HOH:O	2.36	0.82
1:A:196:THR:HG22	6:A:2170:HOH:O	1.80	0.81
1:A:121:LEU:CD2	1:A:228:ILE:HD11	2.15	0.76
1:A:63:PHE:HD2	1:A:68:MET:HE1	1.48	0.76
1:A:368:GLU:HG3	6:A:2232:HOH:O	1.87	0.74
1:B:121:LEU:CD1	1:B:228:ILE:HD11	2.20	0.72
1:B:112:CYS:CB	6:B:2076:HOH:O	2.28	0.71
1:B:172:ARG:HG2	1:B:219:LEU:HD11	1.71	0.71
1:B:379:VAL:HG11	1:B:413:ALA:HA	1.71	0.71
1:A:264:ILE:O	1:A:318:HIS:HE1	1.75	0.69
1:B:145:THR:HG21	1:B:195:TYR:CZ	2.29	0.67
1:A:5:ARG:HD3	6:A:2004:HOH:O	1.94	0.67
1:B:294:HIS:HD2	1:B:295:PRO:O	1.78	0.66
1:A:63:PHE:HD2	1:A:68:MET:CE	2.09	0.65
1:A:34:ILE:HD13	1:B:409:GLN:HB3	1.79	0.65
1:B:271:ILE:HG13	1:B:303:ILE:HD12	1.78	0.65
1:B:42:ASN:HD22	1:B:44:ASN:H	1.44	0.65
1:B:73:GLN:O	1:B:297:THR:HG21	1.97	0.64
1:A:370:ILE:HD11	1:A:380:LEU:HA	1.78	0.63
1:A:299:ASN:HD21	1:B:299:ASN:HD21	1.46	0.63
1:A:68:MET:HA	1:A:68:MET:CE	2.28	0.63
1:B:121:LEU:HD11	1:B:228:ILE:HD11	1.80	0.62
1:A:80:ILE:CD1	1:A:301:LEU:HD13	2.30	0.62
1:B:344:LEU:HD23	1:B:344:LEU:H	1.65	0.62
1:A:283:ARG:HD3	6:A:2192:HOH:O	1.99	0.61
1:A:174:ILE:O	1:A:177:ARG:HD3	2.01	0.61
2:A:1426:BF5:H4	1:B:40:LEU:CD2	2.31	0.61
1:B:369:LEU:HA	1:B:373:LYS:HG3	1.82	0.61
1:B:89:GLN:CG	1:B:93:LYS:HE2	2.26	0.60
1:B:84:LEU:HD11	1:B:113:VAL:HG23	1.84	0.60
1:B:214:LYS:O	1:B:218:GLU:HG3	2.02	0.59
1:A:99:THR:HG22	1:A:109:MET:HB2	1.83	0.59
1:A:101:HIS:HD2	6:A:2068:HOH:O	1.84	0.59
1:B:304:SER:O	1:B:308:HIS:HD2	1.85	0.58
1:B:195:TYR:OH	1:B:230:ASP:OD2	2.17	0.58
1:A:341:LEU:HD22	1:A:414:PHE:HD2	1.69	0.58
1:B:370:ILE:HG13	1:B:398:LEU:HD21	1.85	0.58
1:B:344:LEU:N	1:B:344:LEU:HD23	2.19	0.58
1:B:185:ASN:HD22	1:B:185:ASN:C	2.07	0.58
1:A:2:ASN:HA	6:A:2071:HOH:O	2.03	0.58
1:A:173:ASP:C	1:A:173:ASP:OD1	2.41	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:HB2	1:A:76:PRO:CD	2.33	0.57
1:B:421:ILE:O	1:B:425:LEU:HG	2.04	0.57
1:B:217:TYR:HB2	1:B:249:MET:CE	2.35	0.57
2:A:1426:BF5:H4	1:B:40:LEU:HD21	1.85	0.56
1:A:17:SER:C	1:A:19:ILE:H	2.09	0.56
1:B:84:LEU:CD1	1:B:113:VAL:HG23	2.35	0.55
1:A:89:GLN:HE21	1:A:93:LYS:HG3	1.70	0.55
1:A:68:MET:HA	1:A:68:MET:HE3	1.89	0.55
1:B:42:ASN:ND2	1:B:44:ASN:H	2.04	0.55
1:B:239:ASN:O	1:B:241:PHE:N	2.40	0.54
1:B:218:GLU:CD	6:B:2130:HOH:O	2.46	0.54
1:B:52:VAL:HG22	1:B:62:GLN:NE2	2.21	0.54
2:A:1426:BF5:F1	2:A:1426:BF5:H16A	1.97	0.54
1:A:67:MET:CE	6:A:2201:HOH:O	2.57	0.53
1:B:18:PRO:O	1:B:19:ILE:HB	2.08	0.53
1:B:136:LEU:HD23	1:B:157:ILE:HB	1.91	0.53
1:A:294:HIS:HD2	1:A:295:PRO:O	1.90	0.52
1:A:121:LEU:HD22	1:A:228:ILE:HD11	1.90	0.52
1:B:17:SER:HB2	1:B:18:PRO:O	2.10	0.52
1:A:256:ILE:HD11	1:A:280:LEU:HD13	1.91	0.51
1:A:341:LEU:HD22	1:A:414:PHE:CD2	2.44	0.51
1:A:15:ASN:O	1:B:147:GLN:NE2	2.43	0.51
1:A:369:LEU:HA	1:A:373:LYS:HE2	1.92	0.51
1:A:293:LEU:HD21	1:B:118:GLN:HE21	1.75	0.50
1:A:80:ILE:HD13	1:A:301:LEU:HD13	1.93	0.50
1:A:283:ARG:CD	6:A:2192:HOH:O	2.56	0.50
1:B:367:LYS:HE3	1:B:371:GLU:OE1	2.12	0.50
1:A:63:PHE:CD2	1:A:68:MET:CE	2.93	0.50
1:A:173:ASP:OD1	1:A:174:ILE:N	2.45	0.49
1:B:121:LEU:HD12	1:B:228:ILE:HD11	1.93	0.49
1:B:145:THR:HG21	1:B:195:TYR:OH	2.12	0.49
1:B:2:ASN:ND2	6:B:2173:HOH:O	2.45	0.49
1:A:121:LEU:HD23	1:A:228:ILE:HD11	1.94	0.49
2:A:1426:BF5:F1	2:A:1426:BF5:C16	2.51	0.49
1:B:185:ASN:ND2	1:B:187:GLN:H	2.11	0.48
1:B:121:LEU:HD21	1:B:230:ASP:CG	2.33	0.48
1:B:74:TYR:HA	1:B:294:HIS:CE1	2.48	0.48
1:B:73:GLN:O	1:B:297:THR:CG2	2.60	0.48
1:A:197:VAL:HB	1:A:201:ASN:HD22	1.79	0.48
1:B:337:ALA:O	1:B:341:LEU:HB2	2.14	0.47
1:A:299:ASN:HD21	1:B:299:ASN:ND2	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:HE1	6:B:2012:HOH:O	1.96	0.47
1:B:102:TYR:O	1:B:108:GLN:HB2	2.14	0.47
1:B:264:ILE:HG13	1:B:265:ILE:HG13	1.97	0.46
1:A:42:ASN:OD1	1:A:44:ASN:HB2	2.16	0.46
1:A:99:THR:HG23	1:A:109:MET:N	2.31	0.45
1:B:2:ASN:N	6:B:2003:HOH:O	2.47	0.45
1:A:214:LYS:O	1:A:218:GLU:HG3	2.15	0.45
1:A:95:HIS:HE1	6:A:2185:HOH:O	2.00	0.45
1:B:-1:GLU:O	1:B:105:SER:O	2.34	0.45
1:A:48:PHE:HB2	1:A:72:LEU:HD11	1.99	0.45
1:B:304:SER:O	1:B:308:HIS:CD2	2.69	0.45
1:B:42:ASN:HD21	1:B:44:ASN:HD22	1.65	0.45
1:A:264:ILE:O	1:A:318:HIS:CE1	2.65	0.44
1:A:295:PRO:O	1:A:296:SER:C	2.55	0.44
1:B:77:SER:OG	1:B:289:GLN:HG2	2.17	0.44
1:A:283:ARG:N	1:A:283:ARG:HD2	2.32	0.44
1:A:270:ARG:HD3	1:B:294:HIS:CE1	2.52	0.44
1:A:60:THR:HG22	6:A:2025:HOH:O	2.17	0.44
1:A:313:GLU:CD	1:A:313:GLU:H	2.20	0.44
1:A:68:MET:HE2	1:A:71:ALA:HB3	2.00	0.44
6:A:2007:HOH:O	1:B:150:HIS:HE1	2.01	0.44
1:A:359:LYS:HB2	1:A:397:TYR:CE2	2.53	0.44
1:A:95:HIS:HD2	6:A:2180:HOH:O	2.00	0.43
1:B:75:SER:HB2	1:B:76:PRO:CD	2.48	0.43
1:B:315:PHE:O	1:B:319:VAL:HG12	2.18	0.43
1:A:95:HIS:O	1:A:96:ASN:C	2.57	0.43
1:A:326:TYR:CE1	1:A:354:MET:HE2	2.54	0.43
1:A:33:MET:HG3	1:A:34:ILE:N	2.34	0.42
1:A:49:LYS:HE2	1:B:56:GLU:HB2	2.00	0.42
1:A:339:LYS:HE2	1:A:340:TRP:CZ2	2.54	0.42
1:B:206:ASN:ND2	6:B:2125:HOH:O	2.40	0.42
1:B:294:HIS:NE2	1:B:297:THR:HG22	2.35	0.42
1:B:185:ASN:HD22	1:B:186:PRO:N	2.17	0.41
1:B:65:GLU:HG2	1:B:65:GLU:H	1.60	0.41
1:A:80:ILE:HD12	1:A:301:LEU:HD13	2.01	0.41
1:A:68:MET:HE1	1:A:298:PHE:CE2	2.56	0.41
1:B:366:VAL:HG21	1:B:398:LEU:HG	2.03	0.41
1:B:217:TYR:HB2	1:B:249:MET:HE1	2.02	0.41
1:A:140:PRO:HG2	1:A:204:THR:HG23	2.03	0.41
1:A:368:GLU:CG	6:A:2232:HOH:O	2.59	0.41
1:B:197:VAL:HA	1:B:230:ASP:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:HD22	1:B:414:PHE:CD2	2.56	0.41
1:B:129:ILE:CG2	1:B:154:CYS:HB3	2.51	0.40
1:A:40:LEU:HD21	2:B:1426:BF5:H4	2.02	0.40
1:A:68:MET:HE2	1:A:68:MET:HA	1.99	0.40
1:A:63:PHE:CD2	1:A:68:MET:HE1	2.40	0.40
1:B:341:LEU:HD22	1:B:414:PHE:HD2	1.85	0.40
1:A:91:GLN:NE2	1:A:91:GLN:HA	2.36	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLU:OE1	1:A:211:GLU:OE1[2_565]	1.73	0.47

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	408/425 (96%)	395 (97%)	13 (3%)	0	100	100
1	B	408/425 (96%)	390 (96%)	16 (4%)	2 (0%)	34	30
All	All	816/850 (96%)	785 (96%)	29 (4%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	LYS
1	B	378	GLY

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	358/370 (97%)	338 (94%)	20 (6%)	26	22
1	B	358/370 (97%)	321 (90%)	37 (10%)	9	5
All	All	716/740 (97%)	659 (92%)	57 (8%)	15	11

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	33	MET
1	A	60	THR
1	A	68	MET
1	A	99	THR
1	A	177	ARG
1	A	228	ILE
1	A	263	LYS
1	A	283	ARG
1	A	301	LEU
1	A	307	LEU
1	A	313	GLU
1	A	334	LEU
1	A	341	LEU
1	A	370	ILE
1	A	379	VAL
1	A	380	LEU
1	A	407	PRO
1	A	417	LEU
1	A	420	LEU
1	B	17	SER
1	B	42	ASN
1	B	62	GLN
1	B	65	GLU
1	B	121	LEU
1	B	137	LEU
1	B	145	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	GLU
1	B	178	TRP
1	B	185	ASN
1	B	189	ASN
1	B	219	LEU
1	B	226	LEU
1	B	228	ILE
1	B	241	PHE
1	B	243	VAL
1	B	259	ASP
1	B	280	LEU
1	B	282	GLU
1	B	288	ILE
1	B	297	THR
1	B	307	LEU
1	B	319	VAL
1	B	322	VAL
1	B	334	LEU
1	B	342	THR
1	B	344	LEU
1	B	363	ILE
1	B	368	GLU
1	B	369	LEU
1	B	370	ILE
1	B	373	LYS
1	B	376	LYS
1	B	380	LEU
1	B	381	MET
1	B	417	LEU
1	B	424	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	91	GLN
1	A	95	HIS
1	A	150	HIS
1	A	201	ASN
1	A	237	GLN
1	A	294	HIS
1	A	305	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	318	HIS
1	A	328	ASN
1	B	2	ASN
1	B	42	ASN
1	B	62	GLN
1	B	118	GLN
1	B	150	HIS
1	B	185	ASN
1	B	189	ASN
1	B	201	ASN
1	B	237	GLN
1	B	294	HIS
1	B	299	ASN
1	B	308	HIS
1	B	328	ASN
1	B	348	HIS
1	B	419	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	BF5	A	1426	3	20,29,29	2.96	6 (30%)	20,44,44	1.94	5 (25%)
3	PLP	A	1427	2	15,15,16	0.97	1 (6%)	21,22,23	1.90	3 (14%)
2	BF5	B	1426	3	20,29,29	2.80	6 (30%)	20,44,44	1.72	4 (20%)
3	PLP	B	1427	2	15,15,16	1.05	1 (6%)	21,22,23	1.55	3 (14%)
5	GOL	B	1428	-	5,5,5	0.20	0	5,5,5	0.85	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
2	BF5	A	1426	3	-	0/4/43/43	0/3/4/4
3	PLP	A	1427	2	-	0/6/6/8	0/1/1/1
2	BF5	B	1426	3	-	0/4/43/43	0/3/4/4
3	PLP	B	1427	2	-	0/6/6/8	0/1/1/1
5	GOL	B	1428	-	-	0/4/4/4	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1426	BF5	O2-C12	-4.93	1.25	1.37
2	A	1426	BF5	O2-C12	-4.29	1.27	1.37
3	A	1427	PLP	C3-C2	-2.57	1.39	1.40
2	A	1426	BF5	F1-C1	-2.44	1.33	1.36
3	B	1427	PLP	C3-C2	-2.28	1.39	1.40
2	A	1426	BF5	O1-C3	2.06	1.37	1.35
2	B	1426	BF5	O1-C3	2.44	1.38	1.35
2	B	1426	BF5	C9-N2	2.66	1.43	1.40
2	A	1426	BF5	C2-C1	2.86	1.39	1.36
2	B	1426	BF5	C2-C1	3.47	1.40	1.36
2	B	1426	BF5	C11-C12	4.35	1.48	1.40
2	A	1426	BF5	C11-C12	4.36	1.48	1.40
2	B	1426	BF5	C12-C8	8.95	1.49	1.38
2	A	1426	BF5	C12-C8	10.32	1.50	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1426	BF5	C11-C12-C8	-5.28	117.21	121.68
2	B	1426	BF5	C11-C12-C8	-4.19	118.14	121.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1426	BF5	C13-N1-C2	-3.92	108.41	121.05
2	A	1426	BF5	C13-N1-C2	-3.87	108.55	121.05
2	A	1426	BF5	C16-N1-C2	-2.41	113.26	121.05
3	B	1427	PLP	C6-C5-C4	-2.09	116.37	118.15
2	B	1426	BF5	C16-C15-N3	-2.01	106.70	109.50
3	A	1427	PLP	O2P-P-O1P	2.05	117.18	110.58
2	A	1426	BF5	C14-C13-N1	2.66	116.53	110.49
3	B	1427	PLP	C3-C4-C5	2.75	121.78	118.78
2	B	1426	BF5	C8-C4-C1	2.81	120.58	112.53
2	A	1426	BF5	C8-C4-C1	2.82	120.61	112.53
3	A	1427	PLP	C5A-C5-C4	3.47	126.25	121.65
3	B	1427	PLP	O4P-C5A-C5	3.64	115.01	108.99
3	A	1427	PLP	O4P-C5A-C5	6.05	118.99	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1426	BF5	4	0
2	B	1426	BF5	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 ⓘ

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	412/425 (96%)	0.27	28 (6%) 20 28	11, 22, 52, 69	0
1	B	412/425 (96%)	0.65	49 (11%) 6 8	13, 27, 73, 91	0
All	All	824/850 (96%)	0.46	77 (9%) 11 15	11, 24, 64, 91	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	425	LEU	9.8
1	A	33	MET	6.6
1	B	375	VAL	6.6
1	B	372	GLU	6.3
1	B	377	MET	5.9
1	B	394	PRO	5.8
1	B	379	VAL	5.5
1	B	365	ASP	5.5
1	B	374	ALA	5.4
1	A	376	LYS	5.3
1	A	425	LEU	5.3
1	A	379	VAL	5.3
1	B	369	LEU	4.8
1	B	363	ILE	4.7
1	B	376	LYS	4.7
1	B	241	PHE	4.5
1	B	371	GLU	4.5
1	B	57	ASN	4.4
1	A	392	SER	4.1
1	B	370	ILE	4.1
1	B	424	SER	4.0
1	A	373	LYS	4.0
1	A	370	ILE	4.0
1	B	378	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	392	SER	3.9
1	A	34	ILE	3.7
1	B	373	LYS	3.7
1	A	371	GLU	3.7
1	A	372	GLU	3.7
1	B	33	MET	3.7
1	B	411	ASP	3.7
1	B	408	GLU	3.5
1	A	35	SER	3.5
1	A	380	LEU	3.4
1	B	420	LEU	3.4
1	A	393	ALA	3.3
1	B	239	ASN	3.3
1	B	368	GLU	3.2
1	B	228	ILE	3.1
1	A	374	ALA	3.1
1	A	173	ASP	3.1
1	B	-1	GLU	3.0
1	B	407	PRO	2.9
1	A	377	MET	2.9
1	A	375	VAL	2.9
1	A	368	GLU	2.9
1	B	393	ALA	2.9
1	B	258	ALA	2.8
1	A	367	LYS	2.7
1	A	228	ILE	2.7
1	B	367	LYS	2.7
1	B	412	VAL	2.6
1	B	423	GLU	2.6
1	A	57	ASN	2.6
1	B	34	ILE	2.6
1	B	19	ILE	2.5
1	A	40	LEU	2.5
1	B	364	ASN	2.5
1	A	369	LEU	2.5
1	A	424	SER	2.4
1	B	406	SER	2.4
1	B	59	LYS	2.3
1	A	419	GLN	2.3
1	B	311	GLY	2.3
1	B	195	TYR	2.2
1	A	38	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	226	LEU	2.2
1	B	340	TRP	2.2
1	B	419	GLN	2.1
1	B	121	LEU	2.1
1	A	19	ILE	2.1
1	B	227	ILE	2.1
1	A	18	PRO	2.1
1	B	18	PRO	2.0
1	B	409	GLN	2.0
1	B	178	TRP	2.0
1	B	405	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	BF5	A	1426	26/26	0.85	0.21	1.89	35,40,41,43	0
2	BF5	B	1426	26/26	0.76	0.22	1.04	40,51,52,52	0
3	PLP	A	1427	15/16	0.98	0.16	0.54	18,26,29,29	0
5	GOL	B	1428	6/6	0.80	0.20	0.45	47,49,50,52	0
3	PLP	B	1427	15/16	0.97	0.17	-0.30	20,31,34,34	0
4	IOD	A	1428	1/1	1.00	0.05	-2.57	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.