



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:53 AM GMT

PDB ID : 2PI7
Title : Structure of the catalytic domain of the chick retinal neurite inhibitor-Receptor
Protein Tyrosine Phosphatase CRYP-2/cPTPRO
Authors : Girish, T.S.; Gopal, B.
Deposited on : 2007-04-13
Resolution : 2.59 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>

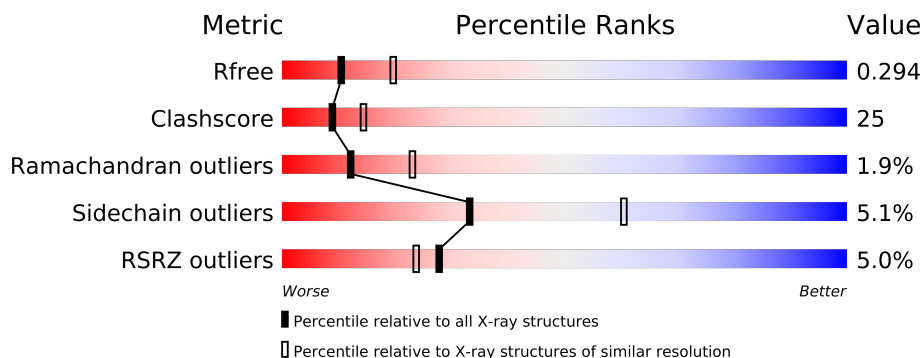
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.59 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	312	
1	B	312	

2 Entry composition i

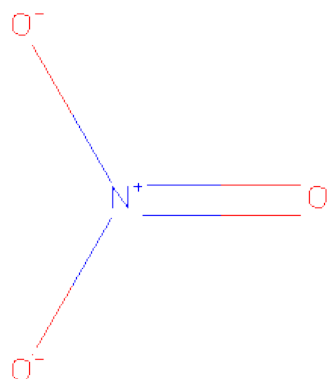
There are 3 unique types of molecules in this entry. The entry contains 4920 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein tyrosine phosphatase CRYP-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2400	1530	408	444	18			
1	B	289	Total	C	N	O	S	0	0	0
			2330	1482	394	436	18			

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is water.

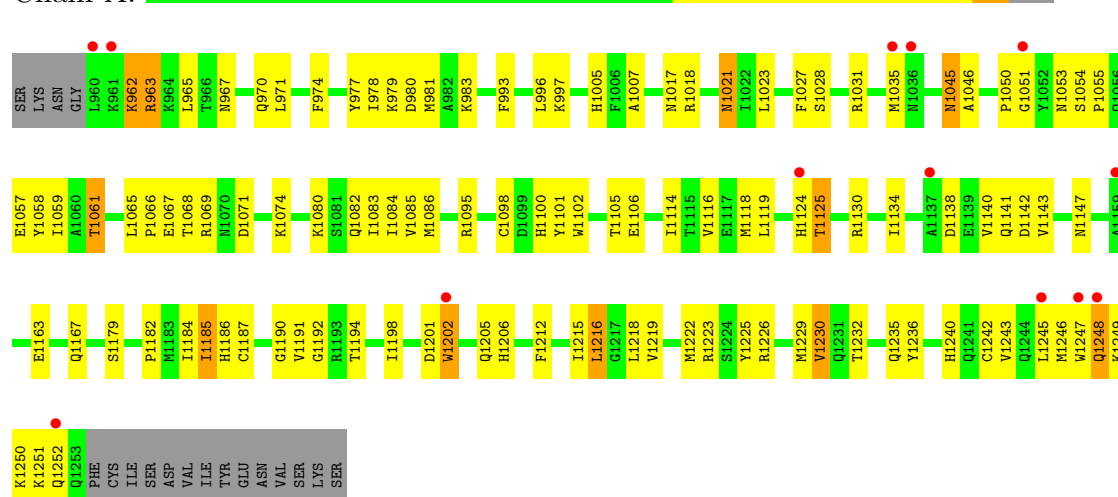
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	0	0
3	B	72	Total 72	O 72	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein tyrosine phosphatase CRYP-2

Chain A:



• Molecule 1: Protein tyrosine phosphatase CRYP-2

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.32Å 68.32Å 245.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.56 – 2.59 19.91 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.56-2.59) 99.4 (19.91-2.61)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.287 0.236 , 0.294	Depositor DCC
R_{free} test set	1063 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 25.0	EDS
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 21002 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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: NO3

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	0.38	0/2461	0.64	0/3334
1	B	0.37	0/2388	0.65	0/3238
All	All	0.38	0/4849	0.65	0/6572

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	2400	0	2307	116	0
1	B	2330	0	2209	119	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	110	0	0	7	0
3	B	72	0	0	9	0
All	All	4920	0	4516	235	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 25.

All (235) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1051:GLY:HA2	1:A:1202:TRP:CZ2	1.77	1.17
1:A:1051:GLY:HA2	1:A:1202:TRP:CH2	1.91	1.05
1:B:1046:ALA:HB2	1:B:1061:THR:HG23	1.38	1.05
1:A:1046:ALA:HB2	1:A:1061:THR:HG23	1.41	1.02
1:A:1202:TRP:CD1	1:A:1218:LEU:HD11	2.00	0.97
1:B:1119:LEU:HD21	1:B:1133:ARG:HB2	1.52	0.92
1:A:1021:ASN:H	1:A:1021:ASN:HD22	1.15	0.87
1:A:1202:TRP:HD1	1:A:1218:LEU:HD11	1.42	0.84
1:A:1105:THR:HG22	1:A:1106:GLU:H	1.41	0.84
1:A:1202:TRP:HZ3	3:A:53:HOH:O	1.60	0.84
1:A:1058:TYR:CE1	1:A:1202:TRP:CH2	2.66	0.84
1:B:1215:ILE:HD11	1:B:1243:VAL:HG21	1.58	0.83
1:A:1058:TYR:HE1	1:A:1202:TRP:CH2	1.96	0.83
1:A:1058:TYR:HE1	1:A:1202:TRP:CZ2	1.96	0.83
1:B:965:LEU:HD23	1:B:999:ILE:HD11	1.59	0.82
1:A:1163:GLU:O	1:A:1167:GLN:HG3	1.79	0.82
1:A:1105:THR:HG22	1:A:1106:GLU:N	1.96	0.80
1:A:1215:ILE:HD11	1:A:1243:VAL:HG21	1.67	0.77
1:B:993:PHE:HA	1:B:996:LEU:HD23	1.67	0.76
1:A:1045:ASN:O	1:A:1061:THR:HG22	1.86	0.75
1:B:1128:VAL:HG21	3:B:19:HOH:O	1.86	0.75
1:A:1051:GLY:CA	1:A:1202:TRP:CH2	2.68	0.75
1:A:1185:ILE:HD11	1:A:1194:THR:HA	1.68	0.75
1:A:1185:ILE:HD11	1:A:1194:THR:HG23	1.69	0.74
1:A:1249:LYS:HA	1:A:1252:GLN:HE21	1.54	0.73
1:A:1046:ALA:CB	1:A:1061:THR:HG23	2.17	0.72
1:B:1119:LEU:HD22	1:B:1119:LEU:H	1.56	0.71
1:A:1050:PRO:O	1:A:1202:TRP:HZ2	1.73	0.71
1:A:1202:TRP:HE3	1:A:1202:TRP:HA	1.57	0.69
1:A:1243:VAL:C	1:A:1245:LEU:H	1.93	0.69
1:A:1021:ASN:HD22	1:A:1021:ASN:N	1.85	0.69
1:B:1243:VAL:C	1:B:1245:LEU:H	1.95	0.69
1:A:965:LEU:HD21	3:A:122:HOH:O	1.93	0.69
1:A:1202:TRP:HA	1:A:1202:TRP:CE3	2.27	0.69
1:B:1165:ILE:H	1:B:1165:ILE:HD12	1.58	0.69
1:A:1084:ILE:HA	1:A:1184:ILE:O	1.92	0.69
1:A:1232:THR:OG1	1:A:1235:GLN:HG3	1.92	0.69
1:A:1105:THR:CG2	1:A:1106:GLU:H	2.07	0.68
1:A:1080:LYS:HA	1:A:1141:GLN:HE22	1.56	0.68
1:A:1116:VAL:HG22	1:A:1134:ILE:HG22	1.76	0.68
1:A:962:LYS:HB3	1:A:962:LYS:HZ3	1.59	0.68
1:B:1123:GLU:HG3	1:B:1128:VAL:HG22	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1239:ILE:O	1:B:1243:VAL:HG23	1.95	0.67
1:B:1119:LEU:HD21	1:B:1133:ARG:CB	2.25	0.67
1:A:1242:CYS:O	1:A:1245:LEU:HG	1.95	0.66
1:B:1077:LEU:HD12	1:B:1141:GLN:NE2	2.10	0.66
1:B:1033:VAL:HB	1:B:1078:GLN:NE2	2.13	0.63
1:B:1185:ILE:HD12	1:B:1197:PHE:CD2	2.33	0.63
1:A:1248:GLN:HE21	1:A:1248:GLN:N	1.96	0.63
1:A:1021:ASN:H	1:A:1021:ASN:ND2	1.92	0.63
1:B:1046:ALA:CB	1:B:1061:THR:HG23	2.22	0.63
1:A:962:LYS:HB3	1:A:962:LYS:NZ	2.14	0.63
1:A:1058:TYR:CE1	1:A:1202:TRP:CZ2	2.85	0.62
1:A:1185:ILE:HD11	1:A:1194:THR:CA	2.30	0.62
1:B:1202:TRP:HE3	3:B:158:HOH:O	1.83	0.62
1:A:1046:ALA:HB2	1:A:1061:THR:CG2	2.24	0.62
1:B:1165:ILE:HD12	1:B:1165:ILE:N	2.15	0.61
1:A:1095:ARG:HG3	1:A:1095:ARG:HH11	1.65	0.61
1:A:1050:PRO:HG2	1:A:1225:TYR:CE2	2.36	0.61
1:B:1021:ASN:HD22	1:B:1021:ASN:H	1.46	0.61
1:A:1067:GLU:CD	1:A:1067:GLU:H	2.04	0.61
1:A:1219:VAL:HA	1:A:1222:MET:HE3	1.81	0.61
1:B:1243:VAL:O	1:B:1243:VAL:HG12	2.01	0.60
1:B:1233:GLU:O	1:B:1237:ILE:HG13	2.00	0.60
1:B:971:LEU:HB3	1:B:1246:MET:HG3	1.84	0.59
1:A:1185:ILE:CD1	1:A:1194:THR:HG23	2.32	0.58
1:B:1157:PRO:HG2	1:B:1241:GLN:HE22	1.69	0.58
1:B:1202:TRP:CE3	1:B:1218:LEU:HD13	2.38	0.58
1:B:1151:TRP:CE2	1:B:1193:ARG:HG2	2.39	0.57
1:B:965:LEU:CD2	1:B:999:ILE:HD11	2.33	0.57
1:A:1246:MET:HG2	1:A:1250:LYS:HD3	1.86	0.57
1:B:998:LEU:O	1:B:1001:LEU:HG	2.05	0.57
1:B:1156:VAL:N	1:B:1234:GLU:OE2	2.38	0.56
1:A:1045:ASN:O	1:A:1061:THR:CG2	2.53	0.56
1:B:1119:LEU:N	1:B:1119:LEU:HD22	2.20	0.56
1:B:992:GLN:O	1:B:996:LEU:HD22	2.05	0.56
1:A:1053:ASN:HD21	1:A:1205:GLN:HE22	1.51	0.56
1:B:1174:GLN:HB3	3:B:77:HOH:O	2.06	0.56
1:B:1123:GLU:HG3	1:B:1128:VAL:CG2	2.35	0.56
1:A:1085:VAL:HB	1:A:1185:ILE:HB	1.88	0.56
1:A:1243:VAL:C	1:A:1245:LEU:N	2.57	0.55
1:B:1082:GLN:HG2	1:B:1142:ASP:O	2.07	0.55
1:B:1008:ALA:HB1	1:B:1023:LEU:HD22	1.87	0.55
1:A:1236:TYR:O	1:A:1240:HIS:HD2	1.90	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1207:ILE:HD12	1:B:1245:LEU:HD12	1.89	0.55
1:B:1151:TRP:CZ2	1:B:1193:ARG:HG2	2.41	0.55
1:A:1017:ASN:ND2	1:A:1045:ASN:HD22	2.05	0.55
1:B:1227:MET:HG2	3:B:61:HOH:O	2.07	0.54
1:B:1236:TYR:O	1:B:1240:HIS:CD2	2.60	0.54
1:B:1185:ILE:HD12	1:B:1197:PHE:HD2	1.72	0.53
1:A:1185:ILE:HD11	1:A:1194:THR:CG2	2.37	0.53
1:A:962:LYS:NZ	1:A:962:LYS:CB	2.71	0.53
1:B:1159:ALA:C	1:B:1161:ALA:N	2.58	0.53
1:A:1018:ARG:NH1	1:A:1065:LEU:HD23	2.24	0.53
1:A:1080:LYS:HA	1:A:1141:GLN:NE2	2.24	0.53
1:B:1033:VAL:HB	1:B:1078:GLN:HE22	1.74	0.53
1:B:1157:PRO:CG	1:B:1241:GLN:HE22	2.22	0.53
1:B:971:LEU:HB3	1:B:1246:MET:CG	2.39	0.53
1:A:1130:ARG:HG3	3:A:64:HOH:O	2.07	0.53
1:A:963:ARG:HG2	1:A:963:ARG:HH11	1.72	0.52
1:B:1157:PRO:HG3	1:B:1238:PHE:CD1	2.44	0.52
1:B:1151:TRP:CD1	1:B:1193:ARG:HD3	2.44	0.52
1:B:990:SER:O	1:B:994:GLU:HB2	2.09	0.52
1:B:980:ASP:HA	1:B:983:LYS:HE3	1.90	0.52
1:A:1185:ILE:CG1	1:A:1194:THR:HG23	2.40	0.52
1:B:1243:VAL:C	1:B:1245:LEU:N	2.63	0.52
1:B:1091:ASN:ND2	1:B:1096:VAL:HA	2.25	0.52
1:B:965:LEU:HB3	1:B:1216:LEU:HD22	1.93	0.51
1:A:1248:GLN:HE21	1:A:1248:GLN:CA	2.22	0.51
1:A:1246:MET:HG2	1:A:1250:LYS:CD	2.40	0.51
1:A:1229:MET:O	1:A:1230:VAL:HB	2.11	0.51
1:A:1138:ASP:O	1:A:1140:VAL:HG23	2.11	0.51
1:A:1031:ARG:HG3	1:A:1031:ARG:HH21	1.74	0.51
1:A:1067:GLU:CD	1:A:1067:GLU:N	2.63	0.51
1:B:1235:GLN:O	1:B:1239:ILE:HG13	2.11	0.50
1:A:1059:ILE:HG13	1:A:1182:PRO:HB2	1.93	0.50
1:A:1095:ARG:NH1	1:A:1095:ARG:HG3	2.24	0.50
1:A:1101:TYR:OH	1:A:1186:HIS:HE1	1.94	0.50
1:B:1021:ASN:ND2	1:B:1021:ASN:H	2.09	0.50
1:A:1240:HIS:HE1	3:A:39:HOH:O	1.95	0.50
1:B:1152:PRO:C	1:B:1154:HIS:H	2.15	0.50
1:B:993:PHE:O	1:B:997:LYS:HG3	2.11	0.50
1:A:979:LYS:HD2	3:A:48:HOH:O	2.12	0.49
1:B:1229:MET:O	1:B:1230:VAL:HB	2.12	0.49
1:A:1243:VAL:O	1:A:1245:LEU:N	2.37	0.49
1:A:1051:GLY:HA2	1:A:1202:TRP:HZ2	1.63	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1165:ILE:O	1:B:1169:VAL:HG23	2.13	0.49
1:B:1249:LYS:O	1:B:1249:LYS:HG2	2.13	0.49
1:B:1151:TRP:O	1:B:1153:ASP:N	2.43	0.49
1:B:1162:ALA:HA	1:B:1165:ILE:HD13	1.94	0.48
1:B:1067:GLU:OE2	1:B:1067:GLU:N	2.46	0.48
1:B:1054:SER:HB2	1:B:1055:PRO:HD2	1.96	0.48
1:A:1202:TRP:CZ3	3:A:53:HOH:O	2.46	0.48
1:A:1105:THR:HG22	1:A:1106:GLU:HG2	1.95	0.48
1:B:1185:ILE:HG21	1:B:1198:ILE:HD11	1.94	0.48
1:B:1074:LYS:O	1:B:1078:GLN:HG3	2.14	0.48
1:A:1124:HIS:CG	1:A:1125:THR:H	2.32	0.48
1:A:1187:CYS:SG	1:A:1190:GLY:HA2	2.54	0.48
1:B:1168:PHE:O	1:B:1172:VAL:HG23	2.14	0.48
1:A:1185:ILE:HD11	1:A:1194:THR:CB	2.44	0.47
1:A:1007:ALA:HB3	3:A:41:HOH:O	2.14	0.47
1:A:1050:PRO:HA	1:A:1055:PRO:HA	1.96	0.47
1:B:1150:ALA:O	1:B:1151:TRP:C	2.52	0.47
1:A:1086:MET:HG2	1:A:1147:ASN:OD1	2.14	0.47
1:A:965:LEU:HB3	1:A:1216:LEU:HD22	1.96	0.47
1:B:994:GLU:HG3	3:B:6:HOH:O	2.14	0.47
1:A:1086:MET:HA	1:A:1186:HIS:O	2.15	0.47
1:A:1191:VAL:HG23	1:A:1192:GLY:N	2.30	0.47
1:B:1185:ILE:HD11	1:B:1197:PHE:HB3	1.95	0.47
1:B:1241:GLN:O	1:B:1244:GLN:HG2	2.15	0.47
1:B:1006:PHE:HA	1:B:1009:ASP:OD2	2.14	0.47
1:A:1251:LYS:O	1:A:1252:GLN:C	2.54	0.46
1:B:1157:PRO:HG3	1:B:1238:PHE:HD1	1.79	0.46
1:A:1074:LYS:HA	1:A:1114:ILE:CD1	2.45	0.46
1:B:1017:ASN:ND2	1:B:1045:ASN:HD22	2.13	0.46
1:B:1128:VAL:HG11	1:B:1130:ARG:NH1	2.31	0.46
1:B:1051:GLY:HA3	1:B:1057:GLU:CB	2.46	0.46
1:B:1212:PHE:CD1	1:B:1212:PHE:C	2.89	0.46
1:A:974:PHE:O	1:A:978:ILE:HG12	2.15	0.46
1:B:1119:LEU:CD2	1:B:1119:LEU:H	2.26	0.46
1:A:1074:LYS:HA	1:A:1114:ILE:HD11	1.98	0.46
1:A:1249:LYS:HA	1:A:1252:GLN:NE2	2.28	0.46
1:B:1091:ASN:HD22	1:B:1096:VAL:HA	1.81	0.46
1:B:1130:ARG:HB2	1:B:1145:HIS:HB3	1.97	0.46
1:A:977:TYR:O	1:A:981:MET:HG2	2.16	0.46
1:A:1223:ARG:HG3	1:A:1229:MET:HB2	1.98	0.45
1:A:1069:ARG:HG3	1:A:1101:TYR:HB2	1.98	0.45
1:A:1202:TRP:CE3	1:A:1202:TRP:CA	2.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:971:LEU:HB3	1:A:1246:MET:SD	2.56	0.45
1:B:1206:HIS:HE1	1:B:1212:PHE:O	1.99	0.45
1:B:1123:GLU:HA	1:B:1128:VAL:HG22	1.98	0.45
1:B:1101:TYR:OH	1:B:1186:HIS:HE1	2.00	0.45
1:B:1158:THR:O	1:B:1159:ALA:O	2.35	0.45
1:B:1128:VAL:CG1	1:B:1130:ARG:NH1	2.79	0.45
1:B:1152:PRO:O	1:B:1154:HIS:N	2.37	0.45
1:B:1040:GLY:HA2	3:B:121:HOH:O	2.17	0.45
1:B:1196:THR:O	1:B:1200:LEU:HG	2.16	0.45
1:A:1066:PRO:HD2	1:A:1067:GLU:OE2	2.17	0.45
1:A:980:ASP:HA	1:A:983:LYS:HG3	1.98	0.45
1:A:1082:GLN:OE1	1:A:1179:SER:HA	2.17	0.45
1:B:1074:LYS:HA	1:B:1114:ILE:CD1	2.46	0.44
1:A:1100:HIS:CD2	1:A:1102:TRP:O	2.70	0.44
1:A:1226:ARG:O	1:A:1229:MET:HG2	2.17	0.44
1:A:1054:SER:O	1:A:1057:GLU:HB2	2.17	0.44
1:B:1026:ASP:CG	3:B:2:HOH:O	2.55	0.44
1:B:975:ASP:O	1:B:979:LYS:HG3	2.18	0.44
1:B:1243:VAL:O	1:B:1243:VAL:CG1	2.65	0.44
1:B:1236:TYR:O	1:B:1240:HIS:HD2	2.00	0.44
1:B:1166:LEU:HD13	1:B:1245:LEU:CD2	2.47	0.44
1:A:1086:MET:HE3	1:A:1101:TYR:HE2	1.83	0.44
1:B:1244:GLN:C	1:B:1246:MET:H	2.21	0.43
1:B:1136:TYR:O	1:B:1137:ALA:C	2.56	0.43
1:B:1151:TRP:HE1	1:B:1154:HIS:CA	2.31	0.43
1:B:1051:GLY:HA3	1:B:1057:GLU:OE1	2.19	0.43
1:B:984:ASP:HB2	1:B:987:TYR:HB2	2.00	0.43
1:B:1158:THR:O	1:B:1159:ALA:C	2.56	0.43
1:A:1018:ARG:NH2	1:A:1098:CYS:HA	2.32	0.43
1:A:1118:MET:SD	1:A:1130:ARG:HD3	2.58	0.43
1:B:1038:GLU:HB3	1:B:1039:GLU:H	1.61	0.43
1:B:1100:HIS:CD2	1:B:1102:TRP:O	2.72	0.43
1:A:1206:HIS:CE1	1:A:1212:PHE:O	2.72	0.43
1:A:1027:PHE:CE2	1:A:1028:SER:HB3	2.54	0.43
1:A:1185:ILE:CD1	1:A:1194:THR:HA	2.46	0.43
1:B:1051:GLY:HA3	1:B:1057:GLU:HB3	2.00	0.43
1:A:993:PHE:O	1:A:997:LYS:HG3	2.19	0.43
1:B:1191:VAL:HG23	1:B:1192:GLY:N	2.34	0.43
1:B:965:LEU:HD22	1:B:965:LEU:N	2.33	0.42
1:B:1248:GLN:C	1:B:1250:LYS:H	2.22	0.42
1:B:1242:CYS:C	1:B:1244:GLN:H	2.22	0.42
1:B:1031:ARG:HG2	3:B:124:HOH:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1119:LEU:HD23	1:A:1119:LEU:C	2.40	0.42
1:B:1116:VAL:HG22	1:B:1134:ILE:HG22	2.02	0.42
1:A:1068:THR:O	1:A:1071:ASP:HB2	2.19	0.41
1:A:1058:TYR:CE1	1:A:1198:ILE:HG23	2.55	0.41
1:B:1108:PRO:HA	1:B:1116:VAL:O	2.19	0.41
1:A:1185:ILE:HG13	1:A:1194:THR:HG23	2.02	0.41
1:B:1021:ASN:N	1:B:1021:ASN:HD22	2.16	0.41
1:A:1083:ILE:HG13	1:A:1179:SER:HB2	2.02	0.41
1:A:1058:TYR:OH	1:A:1201:ASP:OD2	2.29	0.41
1:B:1061:THR:O	1:B:1186:HIS:HB2	2.21	0.41
1:B:1246:MET:O	1:B:1247:TRP:C	2.59	0.41
1:B:1159:ALA:O	1:B:1160:ASN:C	2.58	0.41
1:B:1192:GLY:HA2	1:B:1231:GLN:H	1.85	0.41
1:B:1069:ARG:HD3	1:B:1111:TYR:CE1	2.56	0.41
1:B:1026:ASP:HB3	3:B:2:HOH:O	2.20	0.41
1:A:1005:HIS:CD2	1:A:1023:LEU:HD12	2.55	0.41
1:A:1050:PRO:HG2	1:A:1225:TYR:CZ	2.56	0.40
1:B:1122:GLU:O	1:B:1128:VAL:HG13	2.21	0.40
1:B:1100:HIS:O	1:B:1100:HIS:CD2	2.74	0.40
1:A:1051:GLY:HA3	1:A:1057:GLU:OE1	2.21	0.40
1:B:999:ILE:HD13	1:B:1220:SER:OG	2.21	0.40
1:A:1100:HIS:HD2	1:A:1102:TRP:O	2.04	0.40
1:A:1027:PHE:CG	1:A:1028:SER:N	2.89	0.40
1:B:1165:ILE:CD1	1:B:1165:ILE:H	2.28	0.40
1:B:1185:ILE:HD13	1:B:1194:THR:HG23	2.02	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	292/312 (94%)	261 (89%)	28 (10%)	3 (1%)	22	45
1	B	287/312 (92%)	244 (85%)	35 (12%)	8 (3%)	8	12
All	All	579/624 (93%)	505 (87%)	63 (11%)	11 (2%)	12	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1156	VAL
1	B	1157	PRO
1	B	1158	THR
1	A	1125	THR
1	B	1154	HIS
1	B	1159	ALA
1	B	1177	VAL
1	A	1045	ASN
1	A	1230	VAL
1	B	1230	VAL
1	B	1243	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	261/286 (91%)	246 (94%)	15 (6%)	29	54
1	B	251/286 (88%)	240 (96%)	11 (4%)	39	68
All	All	512/572 (90%)	486 (95%)	26 (5%)	33	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	962	LYS
1	A	963	ARG
1	A	967	ASN
1	A	970	GLN
1	A	996	LEU
1	A	1021	ASN
1	A	1035	MET
1	A	1061	THR
1	A	1142	ASP
1	A	1143	VAL
1	A	1185	ILE
1	A	1202	TRP
1	A	1216	LEU

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Mol	Chain	Res	Type
1	A	1247	TRP
1	A	1248	GLN
1	B	967	ASN
1	B	975	ASP
1	B	1002	ASP
1	B	1021	ASN
1	B	1031	ARG
1	B	1061	THR
1	B	1107	ASP
1	B	1125	THR
1	B	1153	ASP
1	B	1216	LEU
1	B	1246	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	967	ASN
1	A	970	GLN
1	A	992	GLN
1	A	1005	HIS
1	A	1017	ASN
1	A	1021	ASN
1	A	1089	GLN
1	A	1091	ASN
1	A	1100	HIS
1	A	1124	HIS
1	A	1141	GLN
1	A	1154	HIS
1	A	1186	HIS
1	A	1205	GLN
1	A	1206	HIS
1	A	1240	HIS
1	A	1241	GLN
1	A	1248	GLN
1	A	1252	GLN
1	B	967	ASN
1	B	992	GLN
1	B	1017	ASN
1	B	1021	ASN
1	B	1053	ASN
1	B	1091	ASN

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Mol	Chain	Res	Type
1	B	1100	HIS
1	B	1141	GLN
1	B	1174	GLN
1	B	1186	HIS
1	B	1205	GLN
1	B	1206	HIS
1	B	1210	HIS
1	B	1240	HIS
1	B	1241	GLN
1	B	1248	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 ⓘ

2 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	NO3	A	2001	-	3,3,3	0.31	0	3,3,3	0.13	0
2	NO3	B	2002	-	3,3,3	0.47	0	3,3,3	0.09	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	NO3	A	2001	-	-	0/0/0/0	0/0/0/0
2	NO3	B	2002	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/312 (94%)	0.14	13 (4%) 33 29	9, 20, 39, 56	0
1	B	289/312 (92%)	0.33	16 (5%) 24 20	8, 23, 44, 62	0
All	All	583/624 (93%)	0.23	29 (4%) 28 24	8, 21, 42, 62	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	LEU	9.0
1	B	1155	GLY	7.2
1	B	1156	VAL	6.8
1	B	1157	PRO	5.7
1	B	1153	ASP	5.4
1	B	1035	MET	5.3
1	A	1035	MET	4.7
1	B	1137	ALA	4.5
1	B	1158	THR	4.3
1	B	1036	ASN	4.2
1	B	1138	ASP	3.9
1	A	1247	TRP	3.8
1	A	1202	TRP	3.7
1	B	1159	ALA	3.3
1	B	1154	HIS	3.3
1	A	961	LYS	3.3
1	A	1051	GLY	2.8
1	B	1152	PRO	2.7
1	A	1248	GLN	2.7
1	A	1159	ALA	2.4
1	A	1245	LEU	2.3
1	A	1036	ASN	2.3
1	A	1124	HIS	2.2
1	B	1160	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1252	GLN	2.2
1	B	987	TYR	2.2
1	B	1125	THR	2.2
1	A	1137	ALA	2.2
1	B	1124	HIS	2.1

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
2	NO3	A	2001	4/4	0.13	0.23	12,16,17,18	0
2	NO3	B	2002	4/4	0.11	-0.47	21,22,23,25	0

6.5 Other polymers

There are no such residues in this entry.