



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:18 pm BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

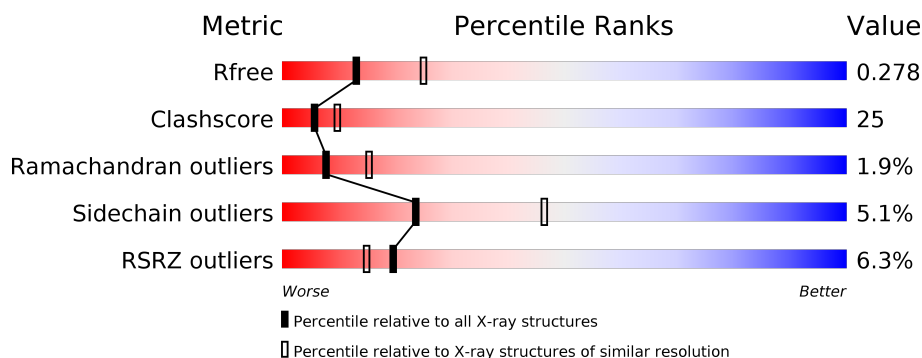
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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  $\geq 3$ , 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	312	<div> <div>5%</div> <div> <div></div> <div>58%</div> <div>33%</div> <div>• 6%</div> </div> </div>
1	B	312	<div> <div>6%</div> <div> <div></div> <div>52%</div> <div>36%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition [i](#)

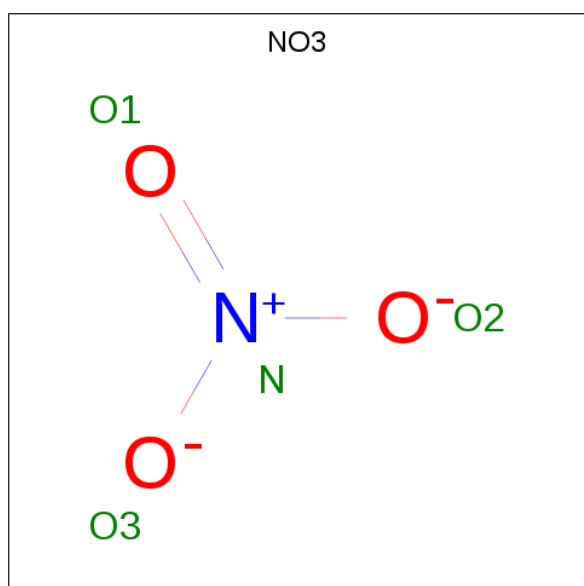
There are 3 unique types of molecules in this entry. The entry contains 4920 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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: NO<sub>3</sub>).



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.287 0.217 , 0.278	Depositor DCC
$R_{free}$ test set	1063 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical 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: 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 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	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

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 25.

All (235) 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: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:1105:THR:HG22	1:A:1106:GLU:H	1.41	0.84
1:A:1202:TRP:HD1	1:A:1218:LEU:HD11	1.42	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:A:965:LEU:HD21	3:A:122:HOH:O	1.93	0.69
1:B:1243:VAL:C	1:B:1245:LEU:H	1.95	0.69
1:A:1202:TRP:CE3	1:A:1202:TRP:HA	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:1116:VAL:HG22	1:A:1134:ILE:HG22	1.76	0.68
1:A:1080:LYS:HA	1:A:1141:GLN:HE22	1.56	0.68
1:A:962:LYS:HB3	1:A:962:LYS:HZ3	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:GLU:HG3	1:B:1128:VAL:HG22	1.75	0.68
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:A:1248:GLN:HE21	1:A:1248:GLN:N	1.96	0.63
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: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:A:1095:ARG:HG3	1:A:1095:ARG:HH11	1.65	0.61
1:B:1165:ILE:N	1:B:1165:ILE:HD12	2.15	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:H	1:A:1067:GLU:CD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1151:TRP:CZ2	1:B:1193:ARG:HG2	2.41	0.55
1:B:1207:ILE:HD12	1:B:1245:LEU:HD12	1.89	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:A:1130:ARG:HG3	3:A:64:HOH:O	2.07	0.53
1:B:971:LEU:HB3	1:B:1246:MET:CG	2.39	0.53
1:A:963:ARG:HH11	1:A:963:ARG:HG2	1.72	0.52
1:B:1151:TRP:CD1	1:B:1193:ARG:HD3	2.44	0.52
1:B:1157:PRO:HG3	1:B:1238:PHE:CD1	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:1091:ASN:ND2	1:B:1096:VAL:HA	2.25	0.52
1:B:1243:VAL:C	1:B:1245:LEU:N	2.63	0.52
1:A:1248:GLN:HE21	1:A:1248:GLN:CA	2.22	0.51
1:B:965:LEU:HB3	1:B:1216:LEU:HD22	1.93	0.51
1:A:1246:MET:HG2	1:A:1250:LYS:CD	2.40	0.51
1:A:1138:ASP:O	1:A:1140:VAL:HG23	2.11	0.51
1:A:1229:MET:O	1:A:1230:VAL:HB	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:A:1240:HIS:HE1	3:A:39:HOH:O	1.95	0.50
1:B:1021:ASN:ND2	1:B:1021:ASN:H	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1067:GLU:OE2	1:B:1067:GLU:N	2.46	0.48
1:B:1162:ALA:HA	1:B:1165:ILE:HD13	1.94	0.48
1:B:1054:SER:HB2	1:B:1055:PRO:HD2	1.96	0.48
1:A:1105:THR:HG22	1:A:1106:GLU:HG2	1.95	0.48
1:A:1202:TRP:CZ3	3:A:53:HOH:O	2.46	0.48
1:B:1185:ILE:HG21	1:B:1198:ILE:HD11	1.94	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:1074:LYS:O	1:B:1078:GLN:HG3	2.14	0.48
1:B:1168:PHE:O	1:B:1172:VAL:HG23	2.14	0.48
1:A:1007:ALA:HB3	3:A:41:HOH:O	2.14	0.47
1:A:1185:ILE:HD11	1:A:1194:THR:CB	2.44	0.47
1:A:1050:PRO:HA	1:A:1055:PRO:HA	1.96	0.47
1:A:1086:MET:HG2	1:A:1147:ASN:OD1	2.14	0.47
1:B:1150:ALA:O	1:B:1151:TRP:C	2.52	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: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:B:1006:PHE:HA	1:B:1009:ASP:OD2	2.14	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:A:1251:LYS:O	1:A:1252:GLN:C	2.54	0.46
1:A:1074:LYS:HA	1:A:1114:ILE:CD1	2.45	0.46
1:B:1157:PRO:HG3	1:B:1238:PHE:HD1	1.79	0.46
1:B:1017:ASN:ND2	1:B:1045:ASN:HD22	2.13	0.46
1:B:1051:GLY:HA3	1:B:1057:GLU:CB	2.46	0.46
1:B:1128:VAL:HG11	1:B:1130:ARG:NH1	2.31	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:A:1074:LYS:HA	1:A:1114:ILE:HD11	1.98	0.46
1:B:1119:LEU:CD2	1:B:1119:LEU:H	2.26	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:A:977:TYR:O	1:A:981:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1130:ARG:HB2	1:B:1145:HIS:HB3	1.97	0.46
1:A:1069:ARG:HG3	1:A:1101:TYR:HB2	1.98	0.45
1:A:1223:ARG:HG3	1:A:1229:MET:HB2	1.98	0.45
1:A:1202:TRP:CE3	1:A:1202:TRP:CA	2.97	0.45
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:1158:THR:O	1:B:1159:ALA:O	2.35	0.45
1:B:1101:TYR:OH	1:B:1186:HIS:HE1	2.00	0.45
1:B:1040:GLY:HA2	3:B:121:HOH:O	2.17	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: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:1082:GLN:OE1	1:A:1179:SER:HA	2.17	0.45
1:A:980:ASP:HA	1:A:983:LYS:HG3	1.98	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:1236:TYR:O	1:B:1240:HIS:HD2	2.00	0.44
1:B:1243:VAL:O	1:B:1243:VAL:CG1	2.65	0.44
1:A:1086:MET:HE3	1:A:1101:TYR:HE2	1.83	0.44
1:B:1166:LEU:HD13	1:B:1245:LEU:CD2	2.47	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:1051:GLY:HA3	1:B:1057:GLU:OE1	2.19	0.43
1:B:1151:TRP:HE1	1:B:1154:HIS:CA	2.31	0.43
1:B:984:ASP:HB2	1:B:987:TYR:HB2	2.00	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:1158:THR:O	1:B:1159:ALA:C	2.56	0.43
1:A:1027:PHE:CE2	1:A:1028:SER:HB3	2.54	0.43
1:A:1206:HIS:CE1	1:A:1212:PHE:O	2.72	0.43
1:B:1100:HIS:CD2	1:B:1102:TRP:O	2.72	0.43
1:A:1185:ILE:CD1	1:A:1194:THR:HA	2.46	0.43
1:A:993:PHE:O	1:A:997:LYS:HG3	2.19	0.43
1:B:1051:GLY:HA3	1:B:1057:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1119:LEU:HD23	1:A:1119:LEU:C	2.40	0.42
1:B:1031:ARG:HG2	3:B:124:HOH:O	2.20	0.42
1:B:1242:CYS:C	1:B:1244:GLN:H	2.22	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:1069:ARG:HD3	1:B:1111:TYR:CE1	2.56	0.41
1:B:1159:ALA:O	1:B:1160:ASN:C	2.58	0.41
1:B:1061:THR:O	1:B:1186:HIS:HB2	2.21	0.41
1:B:1192:GLY:HA2	1:B:1231:GLN:H	1.85	0.41
1:B:1246:MET:O	1:B:1247:TRP:C	2.59	0.41
1:A:1005:HIS:CD2	1:A:1023:LEU:HD12	2.55	0.41
1:B:1026:ASP:HB3	3:B:2:HOH:O	2.20	0.41
1:A:1050:PRO:HG2	1:A:1225:TYR:CZ	2.56	0.40
1:B:1100:HIS:O	1:B:1100:HIS:CD2	2.74	0.40
1:B:1122:GLU:O	1:B:1128:VAL:HG13	2.21	0.40
1:A:1051:GLY:HA3	1:A:1057:GLU:OE1	2.21	0.40
1:A:1100:HIS:HD2	1:A:1102:TRP:O	2.04	0.40
1:B:999:ILE:HD13	1:B:1220:SER:OG	2.21	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%)	15	32
1	B	287/312 (92%)	244 (85%)	35 (12%)	8 (3%)	5	7
All	All	579/624 (93%)	505 (87%)	63 (11%)	11 (2%)	8	15

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%)	20	41
1	B	251/286 (88%)	240 (96%)	11 (4%)	28	53
All	All	512/572 (90%)	486 (95%)	26 (5%)	24	46

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

Mol	Chain	Res	Type
1	A	962	LYS
1	A	963	ARG

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [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](#)

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	B	2002	-	1,3,3	0.30	0	0,3,3	0.00	-
2	NO3	A	2001	-	1,3,3	0.21	0	0,3,3	0.00	-

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.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	294/312 (94%)	0.24	17 (5%)	23 17	9, 20, 39, 56	0
1	B	289/312 (92%)	0.46	20 (6%)	16 12	8, 23, 44, 62	0
All	All	583/624 (93%)	0.35	37 (6%)	20 15	8, 21, 42, 62	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	LEU	9.5
1	B	1156	VAL	8.3
1	B	1155	GLY	8.3
1	B	1035	MET	6.1
1	B	1157	PRO	5.9
1	A	1035	MET	5.7
1	B	1153	ASP	5.5
1	B	1036	ASN	4.8
1	B	1158	THR	4.6
1	B	1137	ALA	4.3
1	A	1247	TRP	4.2
1	B	1138	ASP	4.1
1	A	1202	TRP	3.9
1	B	1159	ALA	3.8
1	B	1154	HIS	3.6
1	B	1152	PRO	3.6
1	A	961	LYS	3.3
1	A	1137	ALA	3.3
1	B	1125	THR	3.0
1	A	1248	GLN	2.9
1	A	1051	GLY	2.8
1	A	1245	LEU	2.8
1	A	1036	ASN	2.8
1	A	1037	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1124	HIS	2.6
1	A	1158	THR	2.6
1	B	1160	ASN	2.5
1	A	1159	ALA	2.5
1	A	1252	GLN	2.4
1	B	1177	VAL	2.4
1	B	1245	LEU	2.4
1	B	1248	GLN	2.3
1	A	1251	LYS	2.3
1	B	1038	GLU	2.2
1	B	987	TYR	2.1
1	B	1140	VAL	2.1
1	A	962	LYS	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NO3	B	2002	4/4	0.98	0.12	21,22,23,25	0
2	NO3	A	2001	4/4	0.98	0.13	12,16,17,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.