



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:14 AM GMT

PDB ID : 3HND  
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effector TTP and substrate GDP  
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.  
Deposited on : 2009-05-31  
Resolution : 3.21 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

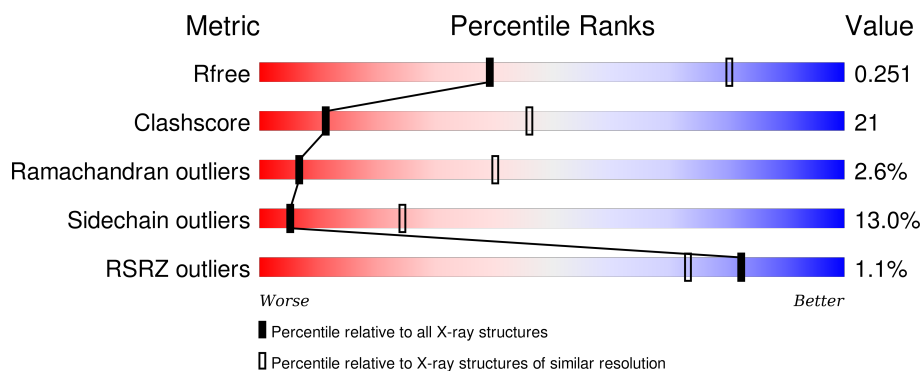
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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. 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	792	
1	B	792	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GDP	A	803	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11566 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.

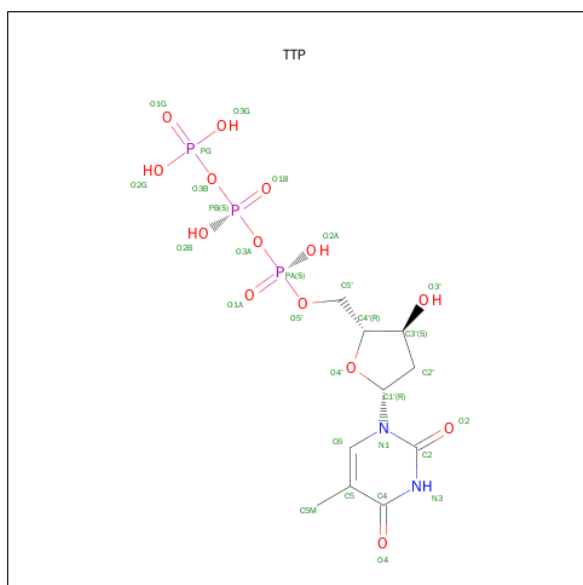
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5720	3640	959	1088	33			
1	B	735	Total	C	N	O	S	0	1	0
			5678	3608	956	1083	31			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

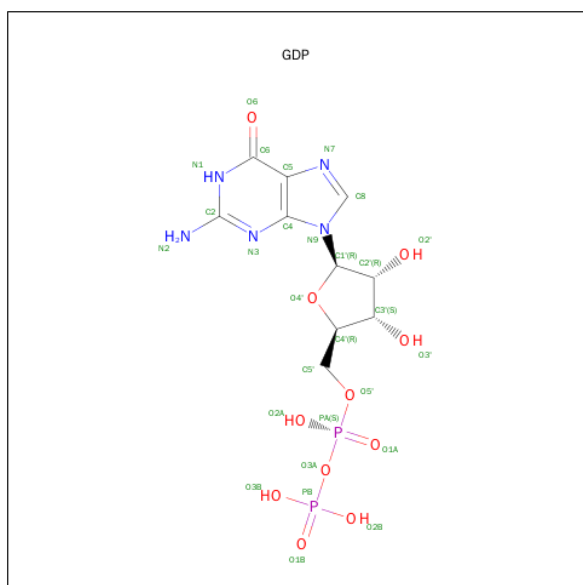
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

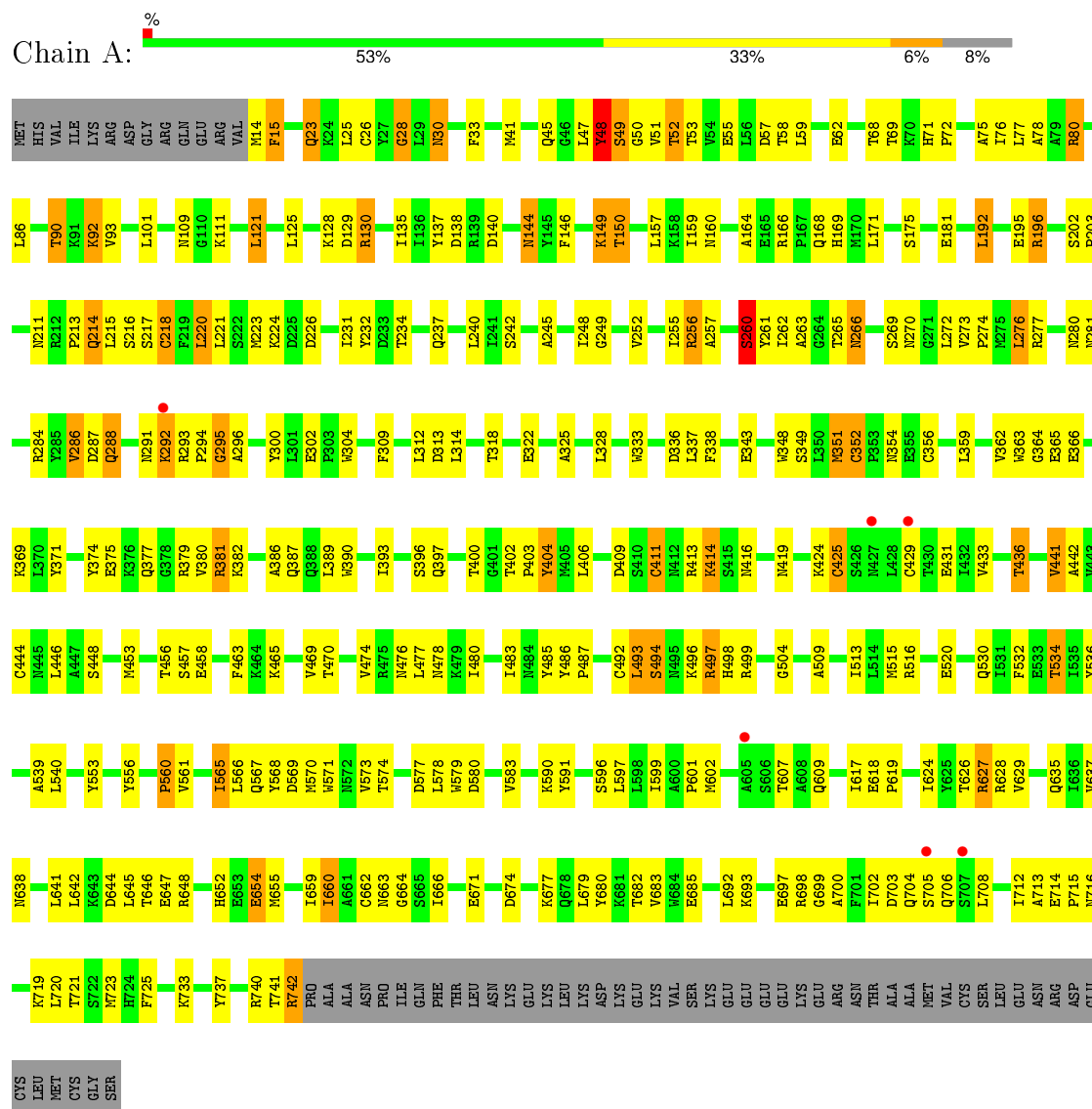
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	14	Total	O	0	0
			14	14		

### 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: Ribonucleoside-diphosphate reductase large subunit



VAL	SER	GLU	GLU	GLU	GLU	GLU	LYS	ARG	ASN	THR	ALA	ALA	MET	GLY	SER
E671	E672	D675	L676	L679	Y680	Q688	V691	L692	K693	E697	R698	F701	Q706	S707	L708
●	●			●											
I565	L566	Y568	W579	D580	W581	K582	L584	K587	K590	Y591	G592	N595	P601	M602	N709
●	●	●				●		●							
I568	L569	Y570	L571	D572	W573	K574	L577	K579	V583	Y584	L586	L589	I593	M594	I710
●	●	●						●							
I596	L597	Y598	L599	D600	W601	K602	L605	K608	V609	Y610	L613	L616	I620	M621	I711
●	●	●						●							
I622	L623	Y624	L627	D628	W629	K630	L633	K636	V637	Y638	L641	L644	I648	M649	I712
●	●	●						●							
I650	L651	Y652	L655	D656	W657	K658	L661	K664	V665	Y666	L669	L672	I676	M677	I713
●	●	●						●							
I684	L685	Y686	L689	D690	W691	K692	L695	K698	V699	Y700	L703	L706	I710	M711	I714
●	●	●						●							
I716	L717	Y718	L721	D722	W723	K724	L727	K730	V731	Y732	L735	L738	I742	M743	I715
●	●	●						●							
I744	L745	Y746	L749	D750	W751	K752	L755	K758	V759	Y760	L763	L766	I770	M771	I716
●	●	●						●							
I772	L773	Y774	L777	D778	W779	K780	L783	K786	V787	Y788	L791	L794	I798	M799	I717
●	●	●						●							
I802	L803	Y804	L807	D808	W809	K810	L813	K816	V817	Y818	L821	L824	I828	M829	I718
●	●	●						●							
I832	L833	Y834	L837	D838	W839	K840	L843	K846	V847	Y848	L851	L854	I858	M859	I719
●	●	●						●							
I862	L863	Y864	L867	D868	W869	K870	L873	K876	V877	Y878	L881	L884	I888	M889	I720
●	●	●						●							
I892	L893	Y894	L897	D898	W899	K900	L903	K906	V907	Y908	L911	L914	I918	M919	I721
●	●	●						●							
I922	L923	Y924	L927	D928	W929	K930	L933	K936	V937	Y938	L941	L944	I948	M949	I722
●	●	●						●							
I952	L953	Y954	L957	D958	W959	K960	L963	K966	V967	Y968	L971	L974	I978	M979	I723
●	●	●						●							
I982	L983	Y984	L987	D988	W989	K990	L993	K996	V997	Y998	L1001	L1004	I1008	M1009	I724
●	●	●						●							
I1012	L1013	Y1014	L1017	D1018	W1019	K1020	L1023	K1026	V1027	Y1028	L1031	L1034	I1038	M1039	I725
●	●	●						●							
I1042	L1043	Y1044	L1047	D1048	W1049	K1050	L1053	K1056	V1057	Y1058	L1061	L1064	I1068	M1069	I726
●	●	●						●							
I1072	L1073	Y1074	L1077	D1078	W1079	K1080	L1083	K1086	V1087	Y1088	L1091	L1094	I1098	M1099	I727
●	●	●						●							
I1102	L1103	Y1104	L1107	D1108	W1109	K1110	L1113	K1116	V1117	Y1118	L1121	L1124	I1128	M1129	I728
●	●	●						●							
I1132	L1133	Y1134	L1137	D1138	W1139	K1140	L1143	K1146	V1147	Y1148	L1151	L1154	I1158	M1159	I729
●	●	●						●							
I1162	L1163	Y1164	L1167	D1168	W1169	K1170	L1173	K1176	V1177	Y1178	L1181	L1184	I1188	M1189	I730
●	●	●						●							
I1192	L1193	Y1194	L1197	D1198	W1199	K1200	L1203	K1206	V1207	Y1208	L1211	L1214	I1218	M1219	I731
●	●	●						●							
I1202	L1203	Y1204	L1207	D1208	W1209	K1210	L1213	K1216	V1217	Y1218	L1221	L1224	I1228	M1229	I732
●	●	●						●							
I1232	L1233	Y1234	L1237	D1238	W1239	K1240	L1243	K1246	V1247	Y1248	L1251	L1254	I1258	M1259	I733
●	●	●						●							
I1242	L1243	Y1244	L1247	D1248	W1249	K1250	L1253	K1256	V1257	Y1258	L1261	L1264	I1268	M1269	I734
●	●	●						●							
I1252	L1253	Y1254	L1257	D1258	W1259	K1260	L1263	K1266	V1267	Y1268	L1271	L1274	I1278	M1279	I735
●	●	●						●							
I1262	L1263	Y1264	L1267	D1268	W1269	K1270	L1273	K1276	V1277	Y1278	L1281	L1284	I1288	M1289	I736
●	●	●						●							
I1272	L1273	Y1274	L1277	D1278	W1279	K1280	L1283	K1286	V1287	Y1288	L1291	L1294	I1298	M1299	I737
●	●	●						●							
I1282	L1283	Y1284	L1287	D1288	W1289	K1290	L1293	K1296	V1297	Y1298	L1301	L1304	I1308	M1309	I738
●	●	●						●							
I1292	L1293	Y1294	L1297	D1298	W1299	K1300	L1303	K1306	V1307	Y1308	L1311	L1314	I1318	M1319	I739
●	●	●						●							
I1302	L1303	Y1304	L1307	D1308	W1309	K1310	L1313	K1316	V1317	Y1318	L1321	L1324	I1328	M1329	I740
●	●	●						●							
I1312	L1313	Y1314	L1317	D1318	W1319	K1320	L1323	K1326	V1327	Y1328	L1331	L1334	I1338	M1339	I741
●	●	●						●							
I1322	L1323	Y1324	L1327	D1328	W1329	K1330	L1333	K1336	V1337	Y1338	L1341	L1344	I1348	M1349	I742
●	●	●						●							
I1332	L1333	Y1334	L1337	D1338	W1339	K1340	L1343	K1346	V1347	Y1348	L1351	L1354	I1358	M1359	I743
●	●	●						●							
I1342	L1343	Y1344	L1347	D1348	W1349	K1350	L1353	K1356	V1357	Y1358	L1361	L1364	I1368	M1369	I744
●	●	●						●							
I1352	L1353	Y1354	L1357	D1358	W1359	K1360	L1363	K1366	V1367	Y1368	L1371	L1374	I1378	M1379	I745
●	●	●						●							
I1362	L1363	Y1364	L1367	D1368	W1369	K1370	L1373	K1376	V1377	Y1378	L1381	L1384	I1388	M1389	I746
●	●	●						●							
I1372	L1373	Y1374	L1377	D1378	W1379	K1380	L1383	K1386	V1387	Y1388	L1391	L1394	I1398	M1399	I747
●	●	●						●							
I1382	L1383	Y1384	L1387	D1388	W1389	K1390	L1393	K1396	V1397	Y1398	L1401	L1404	I1408	M1409	I748
●	●	●						●							
I1392	L1393	Y1394	L1397	D1398	W1399	K1400	L1403	K1406	V1407	Y1408	L1411	L1414	I1418	M1419	I749
●	●	●						●							
I1402	L1403	Y1404	L1407	D1408	W1409	K1410	L1413	K1416	V1417	Y1418	L1421	L1424	I1428	M1429	I750
●	●	●						●							
I1412	L1413	Y1414	L1417	D1418	W1419	K1420	L1423	K1426	V1427	Y1428	L1431	L1434	I1438	M1439	I751
●	●	●						●							
I1422	L1423	Y1424	L1427	D1428	W1429	K1430	L1433	K1436	V1437	Y1438	L1441	L1444	I1448	M1449	I752
●	●	●						●							
I1432	L1433	Y1434	L1437	D1438	W1439	K1440	L1443	K1446	V1447	Y1448	L1451	L1454	I1458	M1459	I753
●	●	●						●							
I1442	L1443	Y1444	L1447	D1448	W1449	K1450	L1453	K1456	V1457	Y1458	L1461	L1464	I1468	M1469	I754
●	●	●						●							
I1452	L1453	Y1454	L1457	D1458	W1459	K1460	L1463	K1466	V1467	Y1468	L1471	L1474	I1478	M1479	I755
●	●	●						●							
I1462	L1463	Y1464	L1467	D1468	W1469	K1470	L1473	K1476	V1477	Y1478	L1481	L1484	I1488	M1489	I756
●	●	●						●							
I1472	L1473	Y1474	L1477	D1478	W1479	K1480	L1483	K1486	V1487	Y1488	L1491	L1494	I1498	M1499	I757
●	●	●						●							
I1482	L1483	Y1484	L1487	D1488	W1489	K1490	L1493	K1496	V1497	Y1498	L1501	L1504	I1508	M1509	I758
●	●	●						●							
I1492	L1493	Y1494	L1497	D1498	W1499	K1500	L1503	K1506	V1507	Y1508	L1511	L1514	I1518	M1519	I759
●	●	●						●							
I1502	L1503	Y1504	L1507	D1508	W1509	K1510	L1513	K1516	V1517	Y1518	L1521	L1524	I1528	M1529	I760
●	●	●						●							
I1512	L1513	Y1514	L1517	D1518	W1519	K1520	L1523	K1526	V1527	Y1528	L1531	L1534	I1538	M1539	I761
●	●	●						●							
I1522	L1523	Y1524	L1527	D1528	W1529	K1530	L1533	K1536	V1537	Y1538	L1541	L1544	I1548	M1549	I762
●	●	●						●							
I1532	L1														



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.16Å 115.83Å 221.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.21 49.92 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.94-3.21) 98.1 (49.92-3.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.180 , 0.254 0.186 , 0.251	Depositor DCC
$R_{free}$ test set	1576 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.0	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 71.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31032 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, TTP, SO4

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	0.61	1/5847 (0.0%)	0.73	0/7950
1	B	0.65	4/5806 (0.1%)	0.74	2/7905 (0.0%)
All	All	0.63	5/11653 (0.0%)	0.73	2/15855 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180[A]	LYS	CG-CD	-7.79	1.25	1.52
1	B	180[B]	LYS	CG-CD	-7.79	1.25	1.52
1	B	129	ASP	CG-OD2	7.36	1.42	1.25
1	B	365	GLU	CB-CG	6.09	1.63	1.52
1	A	411	CYS	CB-SG	-5.01	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ASP	CB-CG-OD1	-7.91	111.18	118.30
1	B	121	LEU	CA-CB-CG	5.70	128.41	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5720	0	5543	239	0
1	B	5678	0	5414	230	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	4	0
3	B	29	0	13	5	0
4	A	28	0	12	2	0
4	B	28	0	12	1	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	18	0	0	4	0
6	B	14	0	0	1	0
All	All	11566	0	11007	465	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 21.

All (465) 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:713:ALA:O	1:A:715:PRO:HD3	1.52	1.09
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.18	1.08
1:A:742:ARG:HA	1:A:742:ARG:NE	1.65	1.04
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.18	1.04
1:A:90:THR:HG21	1:A:166:ARG:HE	1.27	0.99
1:B:106:ASN:HD21	1:B:108:HIS:N	1.61	0.99
1:A:742:ARG:HA	1:A:742:ARG:HE	0.83	0.98
1:B:108:HIS:C	1:B:110:GLY:H	1.60	0.98
1:A:240:LEU:HD23	1:B:228:ILE:HD11	1.47	0.97
1:A:742:ARG:HE	1:A:742:ARG:CA	1.77	0.95
1:A:211:ASN:O	1:A:213:PRO:HD3	1.67	0.94
1:B:106:ASN:HD21	1:B:107:PRO:C	1.72	0.93
1:B:478:ASN:ND2	1:B:499:ARG:HH12	1.68	0.91
1:A:288:GLN:HA	1:A:288:GLN:HE21	1.36	0.90
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.37	0.88
1:A:90:THR:CG2	1:A:166:ARG:HE	1.86	0.88
1:B:52:THR:HB	1:B:55:GLU:HB3	1.56	0.87
1:B:478:ASN:HD21	1:B:499:ARG:NH1	1.72	0.86
1:B:478:ASN:HD21	1:B:499:ARG:HH12	0.88	0.86
1:B:394:ILE:HD11	1:B:717:TYR:HD2	1.40	0.85
1:B:106:ASN:ND2	1:B:107:PRO:C	2.30	0.85
1:B:688:GLN:HA	1:B:691:VAL:HG13	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASN:CG	1:B:107:PRO:N	2.30	0.83
1:B:108:HIS:C	1:B:110:GLY:N	2.30	0.83
1:A:265:THR:O	1:A:266:ASN:HB2	1.78	0.82
1:A:693:LYS:O	1:A:697:GLU:HG3	1.80	0.81
1:A:240:LEU:HD23	1:B:228:ILE:CD1	2.09	0.81
1:B:527:LEU:O	1:B:531:ILE:HG23	1.81	0.81
1:B:106:ASN:ND2	1:B:108:HIS:N	2.30	0.80
1:B:106:ASN:ND2	1:B:107:PRO:N	2.30	0.79
1:A:713:ALA:O	1:A:715:PRO:CD	2.30	0.79
1:B:429:CYS:SG	4:B:803:GDP:H3'	2.22	0.79
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.65	0.78
1:A:30:ASN:HD21	1:A:33:PHE:HD1	1.32	0.78
1:B:221:LEU:HA	1:B:436:THR:HG21	1.65	0.78
1:A:92:LYS:HE2	1:A:92:LYS:H	1.48	0.77
1:A:218:CYS:HB3	4:A:803:GDP:O2'	1.85	0.76
1:A:223:MET:CE	1:A:231:ILE:HA	2.14	0.76
1:A:256:ARG:HG3	1:A:256:ARG:NH1	1.96	0.74
1:A:349:SER:HB2	1:A:380:VAL:CG2	2.17	0.74
1:B:518:PRO:HG2	1:B:521:SER:HB3	1.70	0.74
1:A:90:THR:HG21	1:A:166:ARG:NE	2.02	0.74
1:B:127:ASN:O	1:B:129:ASP:N	2.20	0.74
1:B:394:ILE:CD1	1:B:717:TYR:HD2	2.00	0.74
1:B:530:GLN:O	1:B:534:THR:HG22	1.88	0.73
1:A:256:ARG:CG	1:A:256:ARG:HH11	1.99	0.71
1:B:374:TYR:HE2	1:B:379:ARG:NH1	1.89	0.71
1:A:414:LYS:HB3	1:A:570:MET:HB3	1.73	0.71
1:A:135:ILE:HG21	1:A:137:TYR:CE2	2.25	0.71
1:A:534:THR:HB	1:A:579:TRP:HE1	1.56	0.70
1:A:273:VAL:HG22	1:A:314:LEU:HD21	1.72	0.69
1:B:510:ASP:OD1	1:B:640:HIS:HE1	1.75	0.69
1:B:71:HIS:HD2	1:B:73:ASP:H	1.40	0.69
1:B:394:ILE:HD11	1:B:717:TYR:CD2	2.25	0.69
1:A:476:ASN:O	1:A:480:ILE:HD12	1.93	0.69
1:A:465:LYS:O	1:A:469:VAL:HG23	1.93	0.68
1:B:127:ASN:O	1:B:128:LYS:C	2.30	0.68
1:A:374:TYR:HE2	1:A:379:ARG:HH21	1.40	0.68
1:A:221:LEU:HA	1:A:436:THR:HG21	1.76	0.68
1:A:662:CYS:C	1:A:664:GLY:H	1.97	0.68
1:B:451:LEU:HD22	1:B:531:ILE:HD12	1.75	0.67
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.58	0.67
1:B:109:ASN:O	1:B:110:GLY:C	2.32	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:THR:HB	1:B:403:PRO:HA	1.77	0.67
1:B:709:ASN:OD1	1:B:738:TYR:HB2	1.95	0.67
1:A:429:CYS:SG	4:A:803:GDP:H3'	2.35	0.66
1:A:261:TYR:CE1	1:A:263:ALA:HA	2.30	0.66
1:A:692:LEU:HD23	1:A:708:LEU:HD21	1.78	0.66
1:B:213:PRO:HB2	1:B:215:LEU:HG	1.77	0.66
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.59	0.66
1:A:196:ARG:NH1	1:A:196:ARG:HG2	1.95	0.66
1:A:349:SER:HB2	1:A:380:VAL:HG23	1.77	0.66
1:B:712:ILE:O	1:B:741:THR:HA	1.96	0.66
1:B:256:ARG:HA	1:B:353:PRO:HD2	1.76	0.66
1:B:618:GLU:HB2	1:B:619:PRO:CD	2.26	0.66
1:A:196:ARG:CG	1:A:196:ARG:HH11	2.03	0.65
1:B:83:VAL:HG21	1:B:140:ASP:HB3	1.76	0.65
1:B:693:LYS:O	1:B:697:GLU:HG3	1.96	0.65
1:B:126:ALA:O	1:B:127:ASN:ND2	2.30	0.65
1:A:638:ASN:HD22	1:A:641:LEU:HB2	1.59	0.65
1:A:47:LEU:O	1:A:49:SER:N	2.29	0.65
1:A:402:THR:HB	1:A:403:PRO:HA	1.79	0.65
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.31	0.65
1:B:79:ALA:O	1:B:83:VAL:HG12	1.97	0.65
1:B:109:ASN:O	1:B:111:LYS:N	2.30	0.64
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.78	0.64
1:B:19:THR:HG23	1:B:36:PRO:HB2	1.80	0.64
1:A:456:THR:C	1:A:458:GLU:H	1.99	0.64
1:A:719:LYS:O	1:A:723:MET:HG2	1.98	0.63
1:A:90:THR:CG2	1:A:166:ARG:NE	2.58	0.63
1:B:309:PHE:HB2	6:B:931:HOH:O	1.98	0.63
1:A:220:LEU:N	1:A:220:LEU:CD2	2.61	0.63
1:A:478:ASN:OD1	1:A:499:ARG:NH1	2.31	0.63
1:B:129:ASP:CG	1:B:130:ARG:N	2.52	0.63
1:A:226:ASP:OD2	1:A:256:ARG:NH1	2.31	0.62
1:A:101:LEU:HD13	1:A:157:LEU:HD13	1.81	0.62
1:A:159:ILE:HG22	1:A:160:ASN:HD22	1.64	0.62
1:B:317:ASN:HA	1:B:326:ARG:HE	1.65	0.62
1:A:662:CYS:O	1:A:664:GLY:N	2.33	0.62
1:A:638:ASN:HD22	1:A:641:LEU:CB	2.13	0.62
1:B:635:GLN:O	1:B:636:ILE:HG13	2.00	0.61
1:A:463:PHE:HD2	1:A:534:THR:HG21	1.65	0.61
1:A:601:PRO:HG2	1:A:706:GLN:HB3	1.82	0.60
1:B:84:SER:HA	1:B:87:HIS:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ARG:HD2	1:B:327:ASP:OD2	2.02	0.60
1:A:609:GLN:NE2	1:A:627:ARG:HD3	2.17	0.60
1:B:471:LYS:NZ	1:B:541:GLU:OE1	2.34	0.60
1:B:688:GLN:HA	1:B:691:VAL:CG1	2.31	0.60
1:B:126:ALA:C	1:B:127:ASN:ND2	2.54	0.60
1:A:121:LEU:HD22	1:A:125:LEU:HG	1.83	0.59
1:A:195:GLU:C	1:A:196:ARG:HG3	2.22	0.59
1:B:222:SER:OG	1:B:436:THR:HB	2.02	0.59
1:B:374:TYR:CE2	1:B:379:ARG:NH1	2.69	0.59
1:A:348:TRP:HB2	1:A:386:ALA:HB2	1.83	0.58
1:B:710:ILE:HG22	1:B:739:LEU:HD23	1.84	0.58
1:B:652:HIS:CE1	1:B:655:MET:HB2	2.38	0.58
1:B:618:GLU:HB2	1:B:619:PRO:HD2	1.85	0.58
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.03	0.58
1:B:125:LEU:C	1:B:127:ASN:H	2.06	0.58
1:B:80:ARG:HA	1:B:83:VAL:HG12	1.84	0.58
1:B:221:LEU:HD21	1:B:248:ILE:HG21	1.85	0.58
1:B:534:THR:HB	1:B:579:TRP:HE1	1.67	0.58
1:A:286:VAL:O	1:A:286:VAL:CG2	2.52	0.58
1:B:120:THR:O	1:B:124:VAL:HG23	2.02	0.58
1:B:220:LEU:HD22	1:B:427:ASN:HB3	1.85	0.58
1:A:624:ILE:O	1:A:624:ILE:HD12	2.03	0.58
1:A:702:ILE:HG22	1:A:704:GLN:O	2.03	0.58
1:B:337:LEU:HG	1:B:368:GLU:HG2	1.84	0.58
1:A:292:LYS:O	1:A:293:ARG:HB2	2.03	0.58
1:A:159:ILE:HG12	1:A:164:ALA:HB2	1.85	0.57
1:A:288:GLN:HA	1:A:288:GLN:NE2	2.13	0.57
1:A:530:GLN:O	1:A:534:THR:HG22	2.04	0.57
1:B:159:ILE:O	1:B:159:ILE:HG23	2.05	0.57
1:A:286:VAL:O	1:A:286:VAL:HG22	2.04	0.57
1:B:637:VAL:HG13	1:B:642:LEU:HD22	1.87	0.57
3:A:802:TTP:C5M	1:B:243:LYS:HG3	2.33	0.57
1:A:638:ASN:ND2	1:A:641:LEU:HB2	2.19	0.57
1:B:6:ARG:HD3	1:B:6:ARG:H	1.69	0.57
1:A:14:MET:HG3	1:A:15:PHE:H	1.69	0.57
1:A:256:ARG:HD3	1:A:260:SER:HB3	1.86	0.56
1:A:390:TRP:NE1	1:A:721:THR:HG23	2.20	0.56
1:A:356:CYS:HB3	1:A:374:TYR:CD1	2.39	0.56
1:B:108:HIS:O	1:B:110:GLY:N	2.34	0.56
1:A:570:MET:HE1	6:A:943:HOH:O	2.06	0.56
1:A:652:HIS:CE1	1:A:654:GLU:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:HIS:CD2	1:B:73:ASP:H	2.23	0.56
1:B:602:MET:HG2	1:B:603:PRO:O	2.04	0.56
1:A:260:SER:OG	1:A:352:CYS:SG	2.63	0.56
1:A:221:LEU:HB3	1:A:441:VAL:HB	1.87	0.56
1:B:191:ASN:O	1:B:195:GLU:HB2	2.06	0.56
1:B:86:LEU:HD11	1:B:163:VAL:HG22	1.87	0.56
1:B:298:ALA:HA	1:B:329:PHE:HB2	1.88	0.55
1:B:481:ILE:HD11	1:B:501:ILE:CD1	2.36	0.55
1:B:451:LEU:HD13	1:B:531:ILE:HD11	1.88	0.55
1:B:518:PRO:HD3	1:B:679:LEU:CD2	2.36	0.55
1:A:288:GLN:CA	1:A:288:GLN:HE21	2.16	0.55
1:A:390:TRP:HE1	1:A:721:THR:HG23	1.70	0.55
1:A:232:TYR:OH	1:B:282:THR:HG23	2.06	0.55
1:A:135:ILE:HG21	1:A:137:TYR:CZ	2.41	0.55
1:B:4:ILE:H	1:B:51:VAL:HG13	1.72	0.55
1:B:228:ILE:HD12	1:B:228:ILE:C	2.27	0.55
1:B:130:ARG:CG	1:B:130:ARG:HH11	2.14	0.55
1:A:349:SER:HB2	1:A:380:VAL:HG21	1.86	0.55
1:B:286:VAL:O	1:B:286:VAL:HG22	2.07	0.55
1:B:179:HIS:HD2	1:B:479:LYS:NZ	2.05	0.55
1:B:315:LYS:NZ	1:B:328:LEU:O	2.36	0.55
1:A:402:THR:HG22	1:A:404:TYR:CE1	2.42	0.55
1:A:705:SER:OG	1:A:706:GLN:N	2.38	0.55
1:A:516:ARG:NH2	1:A:644:ASP:OD2	2.30	0.55
1:A:534:THR:HB	1:A:579:TRP:NE1	2.21	0.54
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.88	0.54
1:A:416:ASN:HA	1:A:560:PRO:HG2	1.89	0.54
1:B:125:LEU:C	1:B:127:ASN:N	2.61	0.54
1:B:227:SER:HA	3:B:802:TTP:C5'	2.38	0.54
1:A:90:THR:HG21	1:A:166:ARG:HG2	1.89	0.54
1:A:456:THR:C	1:A:458:GLU:N	2.58	0.54
1:B:504:GLY:HA3	1:B:602:MET:CE	2.37	0.54
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.67	0.53
1:B:518:PRO:HD3	1:B:679:LEU:HD23	1.89	0.53
1:B:117:ALA:HB3	1:B:120:THR:HB	1.90	0.53
1:A:68:THR:OG1	1:A:75:ALA:HB2	2.07	0.53
1:A:362:VAL:HG22	1:A:366:GLU:HB2	1.90	0.53
1:A:213:PRO:HD2	1:A:485:TYR:HB2	1.91	0.53
1:A:699:GLY:HA2	1:A:702:ILE:HD12	1.91	0.53
1:B:242:SER:HB3	1:B:286:VAL:HG22	1.92	0.52
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASN:O	1:B:162:LYS:N	2.41	0.52
1:A:498:HIS:O	1:A:596:SER:HB3	2.09	0.52
1:A:448:SER:HA	1:A:504:GLY:O	2.08	0.52
1:A:240:LEU:CD2	1:B:228:ILE:HD11	2.31	0.52
1:B:292:LYS:HE3	1:B:293:ARG:HH11	1.73	0.52
1:B:280:ASN:HA	1:B:328:LEU:HD21	1.90	0.52
1:B:273:VAL:HG22	1:B:314:LEU:HD21	1.92	0.52
1:B:333:TRP:NE1	1:B:408:LYS:HG3	2.24	0.52
1:A:304:TRP:CZ2	1:A:359:LEU:HB3	2.45	0.52
1:A:431:GLU:OE2	1:A:431:GLU:N	2.43	0.51
1:A:414:LYS:HA	1:A:570:MET:SD	2.50	0.51
1:A:703:ASP:HB3	6:A:942:HOH:O	2.11	0.51
1:A:30:ASN:ND2	1:A:33:PHE:HD1	2.05	0.51
1:B:80:ARG:HA	1:B:83:VAL:CG1	2.40	0.51
1:A:666:ILE:HG23	1:A:677:LYS:HG2	1.92	0.51
1:A:15:PHE:C	1:A:15:PHE:CD2	2.83	0.51
1:A:566:LEU:O	1:A:569:ASP:HB2	2.11	0.51
1:A:364:GLY:N	1:A:409:ASP:OD1	2.38	0.51
1:A:411:CYS:HB3	1:A:433:VAL:HG11	1.92	0.51
1:A:166:ARG:HG3	1:A:169:HIS:CE1	2.46	0.51
1:A:265:THR:O	1:A:266:ASN:CB	2.53	0.51
1:A:601:PRO:HG2	1:A:706:GLN:CB	2.41	0.51
1:B:223:MET:CG	1:B:255:ILE:HD11	2.40	0.51
1:B:602:MET:HE3	1:B:604:THR:HG23	1.92	0.51
1:B:478:ASN:OD1	1:B:595:ASN:ND2	2.39	0.51
1:A:242:SER:HB3	1:A:286:VAL:HG22	1.92	0.51
1:A:565:ILE:HG22	1:A:569:ASP:HB2	1.93	0.51
1:B:93:VAL:HG22	1:B:132:ASN:OD1	2.10	0.51
1:A:213:PRO:O	1:A:215:LEU:HG	2.10	0.50
1:B:126:ALA:C	1:B:127:ASN:HD22	2.14	0.50
1:A:580:ASP:CG	1:A:583:VAL:HG23	2.31	0.50
1:B:676:LEU:HD23	1:B:679:LEU:HD12	1.92	0.50
1:B:36:PRO:O	1:B:39:ILE:HG22	2.11	0.50
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.93	0.50
1:A:72:PRO:HD3	1:A:642:LEU:HD23	1.92	0.50
1:A:272:LEU:O	1:A:276:LEU:HB2	2.12	0.50
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.77	0.50
1:B:40:THR:HG22	1:B:44:ILE:HD12	1.93	0.50
1:B:195:GLU:HB3	1:B:197:TRP:CD1	2.46	0.50
1:A:446:LEU:HB3	1:A:602:MET:CE	2.41	0.50
1:A:226:ASP:OD2	1:A:256:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ASN:ND2	1:A:641:LEU:CB	2.75	0.50
1:B:118:LYS:HG3	1:B:211:ASN:OD1	2.11	0.50
1:A:69:THR:HG22	1:A:635:GLN:O	2.12	0.50
1:B:105:ILE:O	1:B:106:ASN:O	2.30	0.49
1:B:39:ILE:O	1:B:43:VAL:HG23	2.12	0.49
1:B:219:PHE:O	1:B:248:ILE:HA	2.11	0.49
1:B:292:LYS:HE3	1:B:293:ARG:NH1	2.26	0.49
1:A:662:CYS:C	1:A:664:GLY:N	2.66	0.49
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.46	0.49
1:B:484:ASN:OD1	1:B:485:TYR:N	2.45	0.49
1:B:533:GLU:HG2	1:B:701:PHE:CZ	2.48	0.49
1:A:646:THR:C	1:A:648:ARG:H	2.16	0.49
1:B:139:ARG:HD3	1:B:194:SER:OG	2.11	0.49
1:B:500:PRO:O	1:B:501:ILE:HD13	2.12	0.49
1:B:136:ILE:HB	1:B:139:ARG:HD2	1.94	0.49
1:A:76:ILE:O	1:A:80:ARG:HG2	2.11	0.49
1:B:261:TYR:CE1	1:B:263:ALA:HA	2.48	0.49
1:A:343:GLU:HB3	1:A:725:PHE:CE2	2.48	0.49
1:A:414:LYS:HB3	1:A:570:MET:CB	2.43	0.49
1:B:262:ILE:HD12	3:B:802:TTP:O4'	2.12	0.49
1:B:214:GLN:OE1	1:B:244:SER:HB3	2.12	0.48
1:A:477:LEU:HA	1:A:480:ILE:HD13	1.94	0.48
1:B:106:ASN:OD1	1:B:108:HIS:N	2.46	0.48
1:A:90:THR:HG21	1:A:166:ARG:CG	2.44	0.48
1:B:427:ASN:ND2	1:B:429:CYS:H	2.11	0.48
1:A:48:TYR:HA	1:A:51:VAL:HG22	1.95	0.48
1:A:223:MET:HE2	1:A:231:ILE:HA	1.94	0.48
1:B:227:SER:HA	3:B:802:TTP:H5'2	1.95	0.48
1:B:478:ASN:C	1:B:478:ASN:HD22	2.16	0.48
1:A:220:LEU:HD23	1:A:220:LEU:N	2.29	0.48
1:A:712:ILE:O	1:A:741:THR:HG22	2.13	0.48
1:A:86:LEU:O	1:A:90:THR:HB	2.14	0.48
1:A:349:SER:OG	1:A:375:GLU:OE1	2.22	0.48
1:B:3:VAL:HG13	1:B:51:VAL:HA	1.95	0.48
1:A:146:PHE:O	1:A:150:THR:OG1	2.32	0.47
1:A:325:ALA:HB1	1:A:328:LEU:HD12	1.96	0.47
1:A:242:SER:O	1:A:245:ALA:N	2.48	0.47
1:B:299:ILE:HD13	1:B:328:LEU:HD13	1.97	0.47
1:A:416:ASN:OD1	1:A:561:VAL:HG13	2.14	0.47
1:B:111:LYS:O	1:B:113:SER:OG	2.31	0.47
3:A:802:TTP:HM53	1:B:243:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:O	1:B:44:ILE:CG2	2.62	0.47
1:B:481:ILE:HD11	1:B:501:ILE:HD13	1.97	0.46
1:B:6:ARG:HB3	1:B:53:THR:HB	1.97	0.46
1:A:284:ARG:HA	1:A:294:PRO:HB3	1.96	0.46
1:A:513:ILE:HG21	1:A:680:TYR:HE2	1.79	0.46
1:A:617:ILE:H	1:A:617:ILE:HG13	1.59	0.46
1:B:179:HIS:HD2	1:B:479:LYS:HZ3	1.62	0.46
1:B:441:VAL:HG12	1:B:490:GLU:HB2	1.97	0.46
1:A:281:ASN:N	1:A:281:ASN:HD22	2.11	0.46
1:A:396:SER:O	1:A:400:THR:N	2.35	0.46
1:A:77:LEU:O	1:A:78:ALA:C	2.53	0.46
1:B:6:ARG:HD2	1:B:53:THR:HG21	1.97	0.46
1:B:742:ARG:NH1	1:B:742:ARG:HA	2.30	0.46
1:B:18:ILE:O	1:B:22:ILE:HG12	2.16	0.46
1:A:144:ASN:HD22	1:A:144:ASN:H	1.64	0.46
1:A:220:LEU:HB2	1:A:442:ALA:HB3	1.97	0.46
1:B:532:PHE:CD2	1:B:698:ARG:HG3	2.51	0.46
1:B:365:GLU:H	1:B:365:GLU:CD	2.19	0.46
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.82	0.46
1:B:666:ILE:HD11	1:B:680:TYR:HB2	1.98	0.46
1:A:149:LYS:HG2	1:A:629:VAL:HG11	1.98	0.46
1:A:641:LEU:HD21	1:A:666:ILE:HD13	1.97	0.45
1:A:652:HIS:ND1	1:A:654:GLU:HB3	2.31	0.45
1:B:86:LEU:HD11	1:B:163:VAL:CG2	2.46	0.45
1:B:106:ASN:HD21	1:B:108:HIS:CA	2.27	0.45
1:A:49:SER:OG	1:A:49:SER:O	2.30	0.45
1:B:39:ILE:HD11	1:B:64:ALA:HB2	1.98	0.45
1:A:553:TYR:CZ	1:A:556:TYR:HA	2.51	0.45
1:A:211:ASN:O	1:A:213:PRO:CD	2.52	0.45
1:B:149:LYS:HA	1:B:152:GLU:HG2	1.98	0.45
1:A:532:PHE:CE2	1:A:698:ARG:HD3	2.52	0.45
1:B:106:ASN:HD21	1:B:108:HIS:CB	2.30	0.45
1:A:14:MET:HG3	1:A:15:PHE:N	2.30	0.45
1:A:419:ASN:N	1:A:419:ASN:OD1	2.50	0.45
1:A:256:ARG:HG2	1:A:354:ASN:HB2	1.99	0.45
1:B:106:ASN:CG	1:B:108:HIS:N	2.70	0.45
1:B:263:ALA:HB3	3:B:802:TTP:O1G	2.17	0.45
1:B:238:CYS:O	1:B:242:SER:HB2	2.17	0.45
1:A:682:THR:N	1:A:685:GLU:OE1	2.46	0.45
1:A:571:TRP:CD1	1:A:700:ALA:HA	2.52	0.45
1:A:641:LEU:O	1:A:645:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:TYR:CZ	1:A:540:LEU:HD11	2.51	0.45
1:B:130:ARG:NH2	1:B:187:ILE:HD12	2.32	0.45
1:B:109:ASN:C	1:B:111:LYS:N	2.70	0.45
1:B:286:VAL:O	1:B:286:VAL:CG2	2.64	0.45
1:B:225:ASP:OD2	1:B:227:SER:OG	2.23	0.45
1:A:703:ASP:HB2	6:A:941:HOH:O	2.15	0.45
1:B:517:TYR:CE1	1:B:523:GLU:HB3	2.52	0.45
1:B:287:ASP:C	1:B:289:GLY:H	2.21	0.44
1:A:424:LYS:O	1:A:425:CYS:HB3	2.17	0.44
1:B:501:ILE:HD12	1:B:501:ILE:HA	1.66	0.44
1:A:374:TYR:HE2	1:A:379:ARG:NH2	2.11	0.44
1:A:470:THR:O	1:A:474:VAL:HG23	2.17	0.44
1:A:641:LEU:HD13	1:A:680:TYR:CD1	2.53	0.44
1:A:565:ILE:HG23	1:A:569:ASP:HB3	1.99	0.44
1:B:253:SER:OG	1:B:302:GLU:HG3	2.17	0.44
1:B:202:SER:HB2	1:B:203:PRO:HD3	1.99	0.44
1:B:108:HIS:N	1:B:110:GLY:H	2.14	0.44
1:B:121:LEU:HD12	1:B:122:ASP:N	2.33	0.44
1:B:39:ILE:CG2	1:B:40:THR:N	2.80	0.44
1:A:456:THR:O	1:A:458:GLU:N	2.50	0.44
1:B:166:ARG:O	1:B:169:HIS:HB2	2.18	0.44
1:B:518:PRO:CD	1:B:679:LEU:HD23	2.47	0.44
1:B:584:LEU:O	1:B:587:LYS:HG2	2.16	0.44
1:B:221:LEU:CD2	1:B:248:ILE:CG2	2.96	0.44
1:B:650:LEU:HD12	1:B:671:GLU:HB3	2.00	0.44
1:A:742:ARG:CA	1:A:742:ARG:NE	2.51	0.44
1:B:105:ILE:C	1:B:106:ASN:O	2.56	0.44
1:B:108:HIS:H	1:B:110:GLY:H	1.66	0.44
1:A:287:ASP:O	1:A:288:GLN:HB2	2.17	0.44
1:B:123:ILE:O	1:B:126:ALA:HB3	2.17	0.44
1:B:532:PHE:CG	1:B:698:ARG:HG3	2.53	0.44
1:A:109:ASN:HD21	1:A:111:LYS:CB	2.30	0.44
1:B:527:LEU:HG	1:B:527:LEU:O	2.18	0.44
1:A:52:THR:HG23	1:A:55:GLU:OE1	2.18	0.44
1:B:560:PRO:O	1:B:565:ILE:HB	2.18	0.44
1:A:337:LEU:HD21	1:A:371:TYR:HD2	1.82	0.44
1:B:481:ILE:HD11	1:B:501:ILE:HD11	1.98	0.43
1:A:624:ILE:HG12	1:A:660:ILE:HG13	2.00	0.43
1:A:270:ASN:HA	1:A:270:ASN:HD22	1.66	0.43
1:B:566:LEU:HD12	1:B:568:TYR:OH	2.18	0.43
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:TRP:CZ3	1:B:465:LYS:HD3	2.52	0.43
1:B:242:SER:HB3	1:B:286:VAL:CG2	2.48	0.43
1:B:587:LYS:H	1:B:587:LYS:HG2	1.66	0.43
1:B:359:LEU:HA	1:B:359:LEU:HD12	1.82	0.43
1:B:480:ILE:O	1:B:481:ILE:C	2.55	0.43
1:B:675:ASP:O	1:B:679:LEU:HG	2.18	0.43
1:B:95:SER:HB3	1:B:132:ASN:HD21	1.81	0.43
1:B:351:MET:HE3	1:B:371:TYR:CE1	2.53	0.43
1:A:365:GLU:CD	1:A:365:GLU:H	2.21	0.43
1:B:225:ASP:C	1:B:225:ASP:OD2	2.56	0.43
1:A:486:TYR:HA	1:A:487:PRO:HD3	1.82	0.43
1:B:291:ASN:CG	1:B:292:LYS:H	2.22	0.43
1:A:446:LEU:HB3	1:A:602:MET:HE2	2.00	0.43
1:B:220:LEU:N	1:B:220:LEU:HD23	2.34	0.43
1:A:214:GLN:NE2	1:A:216:SER:HB2	2.30	0.43
1:A:363:TRP:CH2	1:A:413:ARG:HA	2.54	0.43
1:A:463:PHE:CE2	1:A:530:GLN:HB3	2.54	0.43
1:A:261:TYR:HE1	1:A:263:ALA:HA	1.80	0.43
1:A:411:CYS:SG	1:A:733:LYS:HB3	2.58	0.43
1:A:683:VAL:C	1:A:685:GLU:H	2.20	0.43
1:B:106:ASN:ND2	1:B:107:PRO:CA	2.81	0.43
1:B:451:LEU:HD11	1:B:505:VAL:HG21	2.01	0.43
1:B:402:THR:HG22	1:B:404:TYR:CE1	2.54	0.43
1:A:638:ASN:ND2	1:A:641:LEU:H	2.16	0.43
1:B:275:MET:CE	1:B:276:LEU:HD13	2.49	0.43
1:A:223:MET:HE3	1:A:234:THR:HB	2.01	0.43
1:B:257:ALA:CB	1:B:306:LEU:HB3	2.49	0.43
1:B:94:PHE:HB2	1:B:135:ILE:CD1	2.49	0.43
1:B:478:ASN:HA	1:B:481:ILE:HD12	2.01	0.42
1:B:121:LEU:C	1:B:123:ILE:N	2.71	0.42
1:A:92:LYS:N	1:A:92:LYS:HE2	2.23	0.42
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.18	0.42
1:A:655:MET:HG2	1:A:659:ILE:HD12	2.01	0.42
1:B:416:ASN:OD1	1:B:561:VAL:HG23	2.19	0.42
1:B:429:CYS:HB2	1:B:431:GLU:OE1	2.19	0.42
1:A:48:TYR:C	1:A:50:GLY:H	2.22	0.42
1:A:23:GLN:C	1:A:25:LEU:H	2.22	0.42
1:A:509:ALA:O	1:A:513:ILE:HG12	2.19	0.42
1:A:402:THR:HG22	1:A:404:TYR:CD1	2.54	0.42
1:B:580:ASP:O	1:B:581:TRP:HB2	2.19	0.42
1:A:248:ILE:HG22	1:A:249:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:HG22	1:B:249:GLY:N	2.34	0.42
1:A:338:PHE:HB2	1:A:348:TRP:CH2	2.55	0.42
1:A:352:CYS:C	1:A:354:ASN:H	2.23	0.42
1:A:337:LEU:CD2	1:A:371:TYR:HD2	2.32	0.42
1:B:544:CYS:HA	1:B:592:GLY:O	2.19	0.42
1:A:202:SER:O	1:A:203:PRO:C	2.57	0.42
1:B:3:VAL:HG22	1:B:51:VAL:HA	2.01	0.42
1:B:638:ASN:HA	1:B:639:PRO:HD3	1.88	0.42
1:B:227:SER:HA	3:B:802:TTP:H5'1	2.02	0.42
1:B:534:THR:HB	1:B:579:TRP:NE1	2.33	0.42
1:B:337:LEU:HD22	1:B:341:ARG:HG2	2.02	0.42
1:B:2:HIS:N	1:B:13:VAL:HG23	2.34	0.42
1:A:351:MET:HG2	1:A:351:MET:H	1.72	0.42
1:A:214:GLN:NE2	1:A:216:SER:H	2.17	0.41
1:A:637:VAL:HB	1:A:642:LEU:HD22	2.01	0.41
1:A:336:ASP:O	1:A:337:LEU:C	2.57	0.41
1:A:256:ARG:NH2	3:A:802:TTP:O3G	2.44	0.41
1:B:451:LEU:HD13	1:B:531:ILE:CD1	2.49	0.41
1:B:348:TRP:HB2	1:B:386:ALA:HB2	2.01	0.41
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.85	0.41
1:B:72:PRO:HD3	1:B:642:LEU:HD23	2.02	0.41
1:A:280:ASN:HD22	1:A:281:ASN:ND2	2.19	0.41
1:A:369:LYS:HB3	1:A:369:LYS:HE2	1.80	0.41
1:B:129:ASP:OD2	1:B:130:ARG:HG3	2.20	0.41
1:B:292:LYS:HB3	1:B:293:ARG:H	1.73	0.41
1:A:26:CYS:O	1:A:28:GLY:N	2.54	0.41
1:B:129:ASP:CG	1:B:130:ARG:H	2.22	0.41
1:A:359:LEU:HA	1:A:359:LEU:HD12	1.81	0.41
1:A:618:GLU:HA	1:A:619:PRO:HD2	1.84	0.41
1:A:352:CYS:SG	1:A:354:ASN:HB3	2.61	0.41
1:A:242:SER:HB3	1:A:286:VAL:CG2	2.51	0.41
1:B:291:ASN:CG	1:B:292:LYS:N	2.73	0.41
1:A:590:LYS:HD3	1:A:591:TYR:CZ	2.56	0.41
1:A:568:TYR:HD2	1:A:573:VAL:O	2.03	0.41
1:A:262:ILE:HD11	1:A:269:SER:HA	2.01	0.41
1:A:713:ALA:HB1	1:A:742:ARG:HG2	2.02	0.41
1:A:257:ALA:O	1:A:260:SER:HB2	2.20	0.41
1:B:130:ARG:HG2	1:B:130:ARG:NH1	2.16	0.41
1:B:510:ASP:OD1	1:B:640:HIS:CE1	2.64	0.41
1:B:244:SER:O	1:B:245:ALA:HB3	2.19	0.41
1:A:192:LEU:HA	1:A:192:LEU:HD12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLY:N	1:B:409:ASP:OD2	2.51	0.41
1:B:44:ILE:O	1:B:44:ILE:HG22	2.20	0.41
1:B:69:THR:HG22	1:B:637:VAL:HG12	2.02	0.41
1:A:280:ASN:HD22	1:A:281:ASN:HD22	1.69	0.41
1:A:381:ARG:HG3	1:A:381:ARG:O	2.21	0.41
1:B:477:LEU:HA	1:B:480:ILE:HD12	2.01	0.41
1:A:223:MET:HE3	1:A:231:ILE:HA	2.00	0.41
1:A:380:VAL:HG22	1:A:382:LYS:H	1.86	0.41
1:B:471:LYS:HG2	1:B:542:ALA:HB2	2.03	0.41
1:A:515:MET:O	1:A:516:ARG:HB2	2.21	0.41
1:B:203:PRO:HG2	1:B:217:SER:HB3	2.03	0.41
1:A:309:PHE:O	1:A:313:ASP:OD1	2.38	0.41
1:A:493:LEU:HD22	1:A:497:ARG:HG3	2.03	0.41
1:A:256:ARG:CD	1:A:260:SER:HB3	2.51	0.41
1:B:73:ASP:HA	1:B:76:ILE:HG13	2.03	0.41
1:B:456:THR:HG22	1:B:458:GLU:H	1.86	0.41
1:B:124:VAL:O	1:B:127:ASN:N	2.53	0.40
1:B:406:LEU:HD22	1:B:426:SER:HB2	2.03	0.40
1:A:220:LEU:N	1:A:220:LEU:HD22	2.35	0.40
1:A:397:GLN:HG2	1:A:403:PRO:HD2	2.02	0.40
1:B:293:ARG:HA	1:B:294:PRO:HD2	1.65	0.40
1:B:351:MET:CE	1:B:371:TYR:CE1	3.04	0.40
1:A:90:THR:HG22	1:A:166:ARG:HE	1.78	0.40
1:A:288:GLN:CA	1:A:288:GLN:NE2	2.79	0.40
1:A:567:GLN:HA	6:A:943:HOH:O	2.21	0.40
1:A:337:LEU:CD2	1:A:371:TYR:CD2	3.04	0.40
1:B:198:PHE:CD2	1:B:199:THR:N	2.90	0.40
1:A:492:CYS:O	1:A:496:LYS:HG2	2.21	0.40
1:A:226:ASP:O	3:A:802:TTP:H5'2	2.20	0.40
1:A:196:ARG:HB2	1:A:453:MET:HE2	2.02	0.40
1:B:650:LEU:HD13	1:B:650:LEU:HA	1.92	0.40
1:A:23:GLN:C	1:A:25:LEU:N	2.75	0.40
1:A:295:GLY:O	1:A:296:ALA:HB3	2.21	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	727/792 (92%)	625 (86%)	84 (12%)	18 (2%)	7	41
1	B	730/792 (92%)	629 (86%)	81 (11%)	20 (3%)	6	39
All	All	1457/1584 (92%)	1254 (86%)	165 (11%)	38 (3%)	7	40

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	TYR
1	A	128	LYS
1	A	224	LYS
1	A	266	ASN
1	A	663	ASN
1	A	714	GLU
1	B	31	MET
1	B	107	PRO
1	B	128	LYS
1	B	161	GLY
1	B	648	ARG
1	A	295	GLY
1	A	457	SER
1	B	109	ASN
1	B	110	GLY
1	B	224	LYS
1	B	718	GLY
1	A	28	GLY
1	A	260	SER
1	A	292	LYS
1	A	377	GLN
1	A	737	TYR
1	B	106	ASN
1	B	292	LYS
1	B	663	ASN

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Mol	Chain	Res	Type
1	A	647	GLU
1	B	160	ASN
1	B	418	GLN
1	A	425	CYS
1	B	91	LYS
1	B	154	SER
1	A	494	SER
1	B	560	PRO
1	B	638	ASN
1	A	393	ILE
1	A	560	PRO
1	B	601	PRO
1	B	636	ILE

### 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	609/693 (88%)	529 (87%)	80 (13%)	5	24
1	B	590/693 (85%)	514 (87%)	76 (13%)	5	24
All	All	1199/1386 (86%)	1043 (87%)	156 (13%)	5	24

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	23	GLN
1	A	30	ASN
1	A	41	MET
1	A	45	GLN
1	A	48	TYR
1	A	49	SER
1	A	52	THR
1	A	53	THR
1	A	57	ASP

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Mol	Chain	Res	Type
1	A	58	THR
1	A	59	LEU
1	A	62	GLU
1	A	80	ARG
1	A	90	THR
1	A	92	LYS
1	A	93	VAL
1	A	121	LEU
1	A	129	ASP
1	A	130	ARG
1	A	138	ASP
1	A	144	ASN
1	A	149	LYS
1	A	150	THR
1	A	171	LEU
1	A	175	SER
1	A	181	GLU
1	A	192	LEU
1	A	196	ARG
1	A	214	GLN
1	A	217	SER
1	A	218	CYS
1	A	220	LEU
1	A	237	GLN
1	A	252	VAL
1	A	256	ARG
1	A	260	SER
1	A	276	LEU
1	A	277	ARG
1	A	286	VAL
1	A	288	GLN
1	A	291	ASN
1	A	312	LEU
1	A	318	THR
1	A	322	GLU
1	A	351	MET
1	A	352	CYS
1	A	381	ARG
1	A	387	GLN
1	A	389	LEU
1	A	404	TYR
1	A	414	LYS

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Mol	Chain	Res	Type
1	A	436	THR
1	A	441	VAL
1	A	444	CYS
1	A	483	ILE
1	A	493	LEU
1	A	494	SER
1	A	497	ARG
1	A	520	GLU
1	A	534	THR
1	A	565	ILE
1	A	574	THR
1	A	577	ASP
1	A	578	LEU
1	A	597	LEU
1	A	599	ILE
1	A	607	THR
1	A	626	THR
1	A	627	ARG
1	A	628	ARG
1	A	654	GLU
1	A	660	ILE
1	A	671	GLU
1	A	674	ASP
1	A	679	LEU
1	A	716	ASN
1	A	720	LEU
1	A	740	ARG
1	A	742	ARG
1	B	6	ARG
1	B	16	ASP
1	B	39	ILE
1	B	59	LEU
1	B	66	THR
1	B	89	GLU
1	B	93	VAL
1	B	99	GLU
1	B	106	ASN
1	B	113	SER
1	B	116	VAL
1	B	118	LYS
1	B	121	LEU
1	B	130	ARG

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Mol	Chain	Res	Type
1	B	138	ASP
1	B	159	ILE
1	B	170	MET
1	B	195	GLU
1	B	217	SER
1	B	220	LEU
1	B	221	LEU
1	B	222	SER
1	B	229	GLU
1	B	250	VAL
1	B	270	ASN
1	B	275	MET
1	B	276	LEU
1	B	286	VAL
1	B	288	GLN
1	B	293	ARG
1	B	301	LEU
1	B	316	LYS
1	B	318	THR
1	B	323	GLN
1	B	337	LEU
1	B	359	LEU
1	B	379	ARG
1	B	383	VAL
1	B	389	LEU
1	B	395	GLU
1	B	398	THR
1	B	436	THR
1	B	439	ASP
1	B	441	VAL
1	B	443	VAL
1	B	445	ASN
1	B	460	THR
1	B	474	VAL
1	B	478	ASN
1	B	483	ILE
1	B	488	VAL
1	B	493	LEU
1	B	494	SER
1	B	501	ILE
1	B	505	VAL
1	B	508	LEU

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Mol	Chain	Res	Type
1	B	531	ILE
1	B	534	THR
1	B	583	VAL
1	B	587	LYS
1	B	590	LYS
1	B	602	MET
1	B	604	THR
1	B	609	GLN
1	B	624	ILE
1	B	637	VAL
1	B	648	ARG
1	B	672	ILE
1	B	691	VAL
1	B	692	LEU
1	B	706	GLN
1	B	707	SER
1	B	708	LEU
1	B	710	ILE
1	B	723	MET
1	B	739	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	160	ASN
1	A	214	GLN
1	A	237	GLN
1	A	268	ASN
1	A	270	ASN
1	A	281	ASN
1	A	288	GLN
1	A	323	GLN
1	A	377	GLN
1	A	613	ASN
1	A	638	ASN
1	A	657	ASN
1	A	724	HIS
1	B	71	HIS
1	B	106	ASN
1	B	127	ASN
1	B	179	HIS

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Mol	Chain	Res	Type
1	B	200	HIS
1	B	237	GLN
1	B	268	ASN
1	B	270	ASN
1	B	346	GLN
1	B	478	ASN
1	B	530	GLN
1	B	595	ASN
1	B	640	HIS
1	B	667	GLN
1	B	678	GLN
1	B	711	HIS
1	B	730	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z  > 2$
3	TTP	A	802	2	21,30,30	0.53	0	31,47,47	1.84	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GDP	A	803	-	23,30,30	1.30	3 (13%)	30,47,47	1.67	6 (20%)
5	SO4	A	805	-	4,4,4	0.16	0	6,6,6	0.41	0
5	SO4	A	806	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	A	807	-	4,4,4	0.12	0	6,6,6	0.16	0
3	TTP	B	802	2	21,30,30	0.56	0	31,47,47	1.86	8 (25%)
4	GDP	B	803	-	23,30,30	1.27	3 (13%)	30,47,47	1.71	5 (16%)
5	SO4	B	804	-	4,4,4	0.23	0	6,6,6	0.27	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
3	TTP	A	802	2	-	0/18/34/34	0/2/2/2
4	GDP	A	803	-	-	0/12/32/32	0/3/3/3
5	SO4	A	805	-	-	0/0/0/0	0/0/0/0
5	SO4	A	806	-	-	0/0/0/0	0/0/0/0
5	SO4	A	807	-	-	0/0/0/0	0/0/0/0
3	TTP	B	802	2	-	0/18/34/34	0/2/2/2
4	GDP	B	803	-	-	0/12/32/32	0/3/3/3
5	SO4	B	804	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	GDP	O4'-C1'	2.06	1.43	1.41
4	B	803	GDP	O4'-C1'	2.60	1.44	1.41
4	B	803	GDP	C6-C5	3.38	1.48	1.41
4	B	803	GDP	C5-C4	3.40	1.48	1.40
4	A	803	GDP	C5-C4	3.55	1.48	1.40
4	A	803	GDP	C6-C5	3.64	1.48	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	TTP	C5-C4-N3	-6.08	118.37	125.14
3	B	802	TTP	C5-C4-N3	-5.11	119.45	125.14
3	B	802	TTP	PB-O3A-PA	-4.19	120.97	132.73
4	B	803	GDP	C5-C6-N1	-3.75	118.47	123.59
4	A	803	GDP	C5-C6-N1	-3.48	118.83	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	GDP	C2'-C1'-N9	-3.29	109.27	114.29
3	A	802	TTP	PB-O3B-PG	-3.23	121.82	132.67
4	B	803	GDP	N3-C2-N1	-3.18	122.60	127.44
4	A	803	GDP	N3-C2-N1	-3.16	122.62	127.44
4	B	803	GDP	C6-C5-C4	-3.08	117.22	120.90
4	A	803	GDP	C6-C5-C4	-2.82	117.52	120.90
3	A	802	TTP	PB-O3A-PA	-2.78	124.93	132.73
4	A	803	GDP	C2'-C1'-N9	-2.41	110.61	114.29
4	A	803	GDP	C4-C5-N7	-2.37	107.30	109.48
3	B	802	TTP	C5M-C5-C4	-2.36	117.00	120.05
3	B	802	TTP	PB-O3B-PG	-2.20	125.30	132.67
3	B	802	TTP	O2G-PG-O3B	2.05	114.40	105.09
3	A	802	TTP	O2B-PB-O3A	2.13	114.73	105.09
3	B	802	TTP	C5M-C5-C6	2.35	123.34	118.62
3	A	802	TTP	O2G-PG-O3B	2.57	116.76	105.09
3	B	802	TTP	O4'-C1'-N1	2.69	112.37	107.72
4	A	803	GDP	C6-N1-C2	4.33	121.95	115.94
3	B	802	TTP	C4-N3-C2	4.52	119.15	115.25
4	B	803	GDP	C6-N1-C2	4.53	122.22	115.94
3	A	802	TTP	C4-N3-C2	4.83	119.42	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	TTP	4	0
4	A	803	GDP	2	0
3	B	802	TTP	5	0
4	B	803	GDP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	729/792 (92%)	-0.07	6 (0%) 87 80	73, 97, 126, 149	0
1	B	735/792 (92%)	-0.15	10 (1%) 78 67	70, 107, 150, 198	0
All	All	1464/1584 (92%)	-0.11	16 (1%) 82 73	70, 101, 145, 198	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	CYS	3.2
1	B	7	ASP	2.7
1	B	291	ASN	2.5
1	B	47	LEU	2.5
1	B	672	ILE	2.5
1	B	10	GLN	2.4
1	A	707	SER	2.4
1	A	705	SER	2.3
1	A	292	LYS	2.3
1	B	48	TYR	2.3
1	A	605	ALA	2.2
1	B	679	LEU	2.2
1	B	290	GLY	2.2
1	B	624	ILE	2.2
1	B	69	THR	2.1
1	A	427	ASN	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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	806	5/5	0.79	0.32	1.97	162,163,163,163	0
4	GDP	A	803	28/28	0.94	0.47	1.79	106,109,109,109	0
4	GDP	B	803	28/28	0.90	0.25	0.90	113,115,119,119	0
3	TTP	B	802	29/29	0.98	0.16	-0.90	65,76,83,85	0
3	TTP	A	802	29/29	0.97	0.15	-1.16	75,82,92,94	0
5	SO4	B	804	5/5	0.95	0.15	-	153,153,153,153	0
2	MG	B	801	1/1	0.95	0.23	-	73,73,73,73	0
5	SO4	A	805	5/5	0.97	0.17	-	99,99,100,100	0
2	MG	A	801	1/1	0.96	0.23	-	92,92,92,92	0
5	SO4	A	807	5/5	0.90	0.12	-	153,153,153,154	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.