



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

PDB ID : 2F95  
Title : M intermediate structure of sensory rhodopsin II/transducer complex in combination with the ground state structure  
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Deposited on : 2005-12-05  
Resolution : 2.20 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

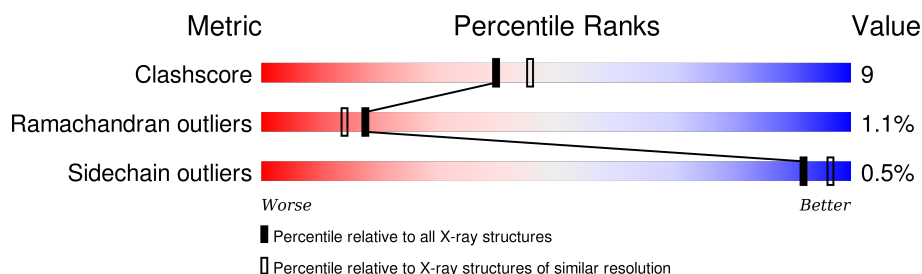
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1-A	248	
1	2-A	248	
2	1-B	163	
2	2-B	163	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4183 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 Sensory rhodopsin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	220	Total	C	N	O	S	0	220	0
			1664	1113	264	281	6			
1	2-A	220	Total	C	N	O	S	0	220	0
			1664	1113	264	281	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLU	-	CLONING ARTIFACT	UNP P42196
A	241	ASN	-	CLONING ARTIFACT	UNP P42196
A	242	SER	-	CLONING ARTIFACT	UNP P42196
A	243	HIS	-	EXPRESSION TAG	UNP P42196
A	244	HIS	-	EXPRESSION TAG	UNP P42196
A	245	HIS	-	EXPRESSION TAG	UNP P42196
A	246	HIS	-	EXPRESSION TAG	UNP P42196
A	247	HIS	-	EXPRESSION TAG	UNP P42196
A	248	HIS	-	EXPRESSION TAG	UNP P42196
A	249	HIS	-	EXPRESSION TAG	UNP P42196

- Molecule 2 is a protein called Sensory rhodopsin II transducer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1-B	53	Total	C	N	O	0	53	0
			356	235	55	66			
2	2-B	53	Total	C	N	O	0	53	0
			356	235	55	66			

There are 10 discrepancies between the modelled and reference sequences:

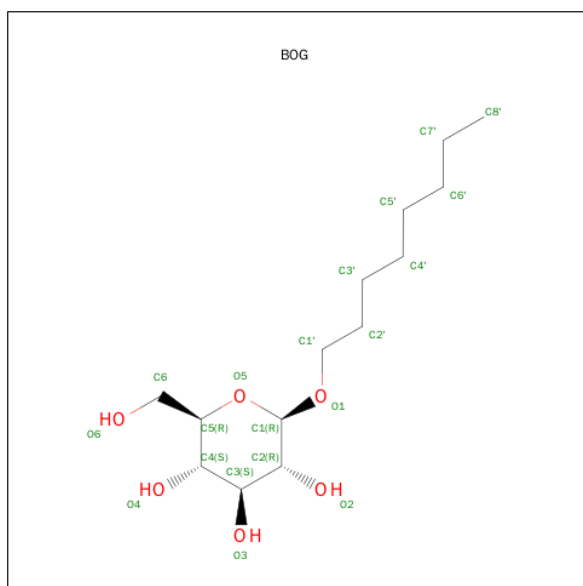
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ALA	-	CLONING ARTIFACT	UNP P42259
B	158	ASN	-	CLONING ARTIFACT	UNP P42259

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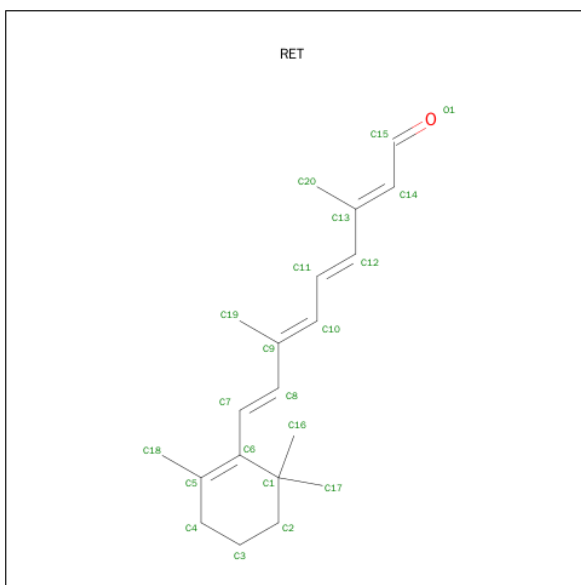
Chain	Residue	Modelled	Actual	Comment	Reference
B	159	SER	-	CLONING ARTIFACT	UNP P42259
B	160	HIS	-	EXPRESSION TAG	UNP P42259
B	161	HIS	-	EXPRESSION TAG	UNP P42259
B	162	HIS	-	EXPRESSION TAG	UNP P42259
B	163	HIS	-	EXPRESSION TAG	UNP P42259
B	164	HIS	-	EXPRESSION TAG	UNP P42259
B	165	HIS	-	EXPRESSION TAG	UNP P42259
B	166	HIS	-	EXPRESSION TAG	UNP P42259

- Molecule 3 is M intermediate of sensory rhodopsin II (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	1
			20	14	6		
3	2-A	1	Total	C	O	0	1
			20	14	6		

- Molecule 4 is RETINAL (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	1	Total C 20 20	0	1
4	2-A	1	Total C 20 20	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	32	Total O 32 32	0	32
5	2-A	28	Total O 28 28	0	28
5	1-B	1	Total O 1 1	0	1
5	2-B	2	Total O 2 2	0	2



ALA	VAL	SER	ARG	SER	ARG	GLY	SER	MET	ARG	LEU	ASP	GLY	LEU	ASP	LEU	PRO	SER	ASP	VAL	ARG	VAL	ARG	GLU	THR	SER	THR	GLN	ASP	GLY	LYS	PHE	VAL	ALA	PHE	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	127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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.62Å 46.90Å 53.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.01 – 2.20	Depositor
% Data completeness (in resolution range)	94.0 (22.01-2.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, BOG

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	1-A	0.35	0/1706	0.54	0/2335
2	1-B	0.26	0/358	0.45	0/490
All	All	0.34	0/2064	0.52	0/2825

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	1-A	1664	0	1730	16	0
1	2-A	1664	0	1731	48	0
2	1-B	356	0	381	3	0
2	2-B	356	0	381	7	0
3	1-A	20	0	28	5	0
3	2-A	20	0	28	3	0
4	1-A	20	0	27	1	0
4	2-A	20	0	27	1	0
5	1-A	32	0	0	0	0
5	1-B	1	0	0	0	0
5	2-A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2-B	2	0	0	1	0
All	All	4183	0	4333	74	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 9.

All (74) 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:66[B]:ARG:HD3	1:A:182[B]:PRO:O	1.69	0.93
1:A:31[B]:SER:O	1:A:33[B]:GLU:N	2.13	0.80
1:A:185[B]:VAL:HG23	1:A:187[B]:LEU:HG	1.66	0.77
1:A:213[A]:LEU:HD12	3:A:300[A]:BOG:H8'1	1.70	0.74
1:A:142[B]:VAL:O	1:A:146[B]:THR:HB	1.91	0.70
1:A:6[B]:THR:O	1:A:10[B]:LEU:HG	1.92	0.70
2:B:30[A]:GLY:O	2:B:34[A]:VAL:HG23	1.99	0.62
1:A:190[B]:PRO:O	1:A:194[B]:VAL:HG23	2.00	0.62
1:A:149[B]:ALA:C	1:A:157[B]:LYS:HD3	2.21	0.61
1:A:162[B]:ARG:HD2	1:A:211[B]:ILE:CG2	2.31	0.60
1:A:37[A]:TYR:CE1	3:A:300[A]:BOG:H8'2	2.37	0.59
1:A:68[B]:VAL:HG21	1:A:116[B]:ALA:O	2.03	0.59
1:A:199[B]:TYR:O	1:A:203[B]:VAL:HG23	2.06	0.56
1:A:61[A]:VAL:HG12	1:A:63[A]:VAL:HG23	1.88	0.56
1:A:149[B]:ALA:O	1:A:157[B]:LYS:HD3	2.05	0.56
1:A:64[B]:ALA:O	1:A:65[B]:GLU:HB2	2.06	0.55
1:A:63[A]:VAL:O	1:A:66[A]:ARG:HG2	2.07	0.55
1:A:152[B]:ARG:HH22	3:A:300[B]:BOG:H62	1.72	0.55
1:A:80[A]:THR:N	1:A:81[A]:PRO:HD2	2.23	0.54
1:A:31[B]:SER:C	1:A:33[B]:GLU:H	2.11	0.53
1:A:192[A]:VAL:HG13	2:B:36[A]:PHE:HZ	1.73	0.53
1:A:141[B]:LEU:HD23	1:A:145[B]:MET:SD	2.50	0.52
1:A:143[B]:GLY:O	1:A:147[B]:GLU:HG3	2.10	0.52
1:A:164[B]:ARG:NH1	1:A:165[B]:ASN:OD1	2.42	0.52
1:A:90[B]:LEU:O	1:A:152[B]:ARG:HD3	2.11	0.51
1:A:162[B]:ARG:HD2	1:A:211[B]:ILE:HG23	1.92	0.51
1:A:13[B]:ILE:O	1:A:17[B]:VAL:HG23	2.10	0.50
1:A:213[A]:LEU:HD12	3:A:300[A]:BOG:C8'	2.41	0.50
1:A:190[B]:PRO:HD2	5:B:167[B]:HOH:O	2.12	0.50
1:A:37[A]:TYR:CZ	3:A:300[A]:BOG:H8'2	2.47	0.49
1:A:74[B]:ILE:HD11	1:A:113[B]:PHE:CE2	2.48	0.49
2:B:57[B]:GLN:O	2:B:61[B]:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31[B]:SER:C	1:A:33[B]:GLU:N	2.66	0.47
1:A:70[B]:ALA:O	1:A:74[B]:ILE:HG12	2.15	0.47
1:A:101[B]:VAL:HG11	1:A:145[B]:MET:SD	2.54	0.47
1:A:185[B]:VAL:CG2	1:A:187[B]:LEU:HG	2.41	0.47
2:B:29[A]:VAL:HG23	2:B:30[A]:GLY:N	2.30	0.47
2:B:40[B]:ALA:HB1	2:B:63[B]:ALA:CB	2.44	0.47
1:A:80[B]:THR:N	1:A:81[B]:PRO:HD2	2.31	0.46
1:A:9[B]:TRP:CE2	1:A:55[B]:ALA:HB1	2.51	0.46
1:A:200[B]:LEU:O	1:A:204[B]:THR:HG23	2.16	0.46
1:A:88[B]:GLY:HA3	1:A:98[B]:PHE:CE1	2.52	0.45
1:A:93[A]:LEU:HD21	1:A:145[A]:MET:HG2	1.98	0.45
1:A:101[A]:VAL:HG11	1:A:145[A]:MET:SD	2.57	0.45
1:A:4[B]:LEU:HD22	1:A:194[B]:VAL:HG21	1.99	0.45
1:A:194[B]:VAL:O	1:A:198[B]:VAL:HG23	2.16	0.45
1:A:34[B]:ARG:O	1:A:38[B]:VAL:HG23	2.17	0.45
1:A:42[B]:GLY:O	1:A:46[B]:ILE:HG13	2.17	0.45
2:B:40[B]:ALA:O	2:B:44[B]:VAL:HG23	2.17	0.44
4:A:301[A]:RET:H181	4:A:301[A]:RET:H7	1.85	0.44
1:A:93[B]:LEU:HB3	1:A:97[B]:GLU:HB2	1.99	0.44
1:A:53[B]:VAL:HG13	1:A:58[B]:VAL:HB	1.99	0.44
1:A:34[B]:ARG:HD2	1:A:38[B]:VAL:HG23	2.00	0.43
1:A:182[B]:PRO:HB2	1:A:183[B]:PRO:HD3	2.00	0.43
1:A:135[B]:LEU:HD23	1:A:135[B]:LEU:HA	1.81	0.43
1:A:187[A]:LEU:HD23	1:A:187[A]:LEU:HA	1.88	0.43
1:A:36[B]:TYR:CE2	3:A:300[B]:BOG:H3'2	2.54	0.43
1:A:97[B]:GLU:O	1:A:101[B]:VAL:HG22	2.19	0.43
1:A:118[B]:VAL:O	1:A:123[B]:ARG:HD3	2.20	0.42
2:B:40[B]:ALA:HB1	2:B:63[B]:ALA:HB1	2.02	0.42
2:B:75[B]:LEU:HD12	2:B:75[B]:LEU:HA	1.95	0.42
1:A:70[B]:ALA:N	1:A:71[B]:PRO:CD	2.83	0.42
1:A:33[B]:GLU:HG3	3:A:300[B]:BOG:H4'1	2.01	0.42
4:A:301[B]:RET:H8	4:A:301[B]:RET:H161	2.01	0.42
1:A:75[A]:ASP:OD1	1:A:75[A]:ASP:C	2.58	0.41
1:A:194[A]:VAL:O	1:A:198[A]:VAL:HG23	2.20	0.41
1:A:192[B]:VAL:HG13	2:B:36[B]:PHE:HZ	1.85	0.41
1:A:212[A]:ALA:HB1	3:A:300[A]:BOG:H7'1	2.03	0.41
2:B:74[B]:ASN:O	2:B:78[B]:VAL:HG23	2.21	0.41
1:A:143[B]:GLY:HA3	1:A:144[B]:PRO:HD3	1.92	0.41
1:A:72[A]:ARG:O	1:A:75[A]:ASP:HB3	2.21	0.41
1:A:142[B]:VAL:O	1:A:146[B]:THR:CB	2.65	0.41
1:A:167[A]:THR:HG23	1:A:171[A]:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[B]:PHE:CZ	1:A:209[B]:GLY:HA3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	1-A	218/248 (88%)	215 (99%)	2 (1%)	1 (0%)	34	35
1	2-A	218/248 (88%)	205 (94%)	8 (4%)	5 (2%)	8	4
2	1-B	51/163 (31%)	50 (98%)	1 (2%)	0	100	100
2	2-B	51/163 (31%)	48 (94%)	3 (6%)	0	100	100
All	All	538/822 (66%)	518 (96%)	14 (3%)	6 (1%)	17	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	31[B]	SER
1	2-A	32[B]	GLY
1	2-A	120[B]	GLY
1	2-A	143[B]	GLY
1	1-A	64[A]	ALA
1	2-A	153[B]	SER

### 5.3.2 Protein sidechains [i](#)

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	1-A	167/189 (88%)	166 (99%)	1 (1%)	90	95
2	1-B	32/120 (27%)	32 (100%)	0	100	100
All	All	199/309 (64%)	198 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	66[A]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	1-B	74[A]	ASN

### 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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BOG	1-A	300[A]	-	20,20,20	1.00	2 (10%)	25,25,25	0.66	0
4	RET	1-A	301[A]	1	19,20,21	1.57	4 (21%)	27,27,28	2.30	11 (40%)
3	BOG	2-A	300[B]	-	20,20,20	1.00	2 (10%)	25,25,25	0.66	0
4	RET	2-A	301[B]	-	19,20,21	1.82	6 (31%)	27,27,28	2.41	12 (44%)

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	BOG	1-A	300[A]	-	-	0/11/31/31	0/1/1/1
4	RET	1-A	301[A]	1	-	0/13/30/31	0/1/1/1
3	BOG	2-A	300[B]	-	-	0/11/31/31	0/1/1/1
4	RET	2-A	301[B]	-	-	0/13/30/31	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-A	301[A]	RET	C16-C1	2.06	1.58	1.53
4	2-A	301[B]	RET	C8-C7	2.07	1.39	1.33
4	2-A	301[B]	RET	C11-C12	2.32	1.40	1.34
3	1-A	300[A]	BOG	O5-C1	2.44	1.48	1.41
3	2-A	300[B]	BOG	O5-C1	2.44	1.48	1.41
4	2-A	301[B]	RET	C10-C9	2.47	1.39	1.35
4	2-A	301[B]	RET	C17-C1	2.56	1.59	1.53
3	1-A	300[A]	BOG	C4-C5	2.60	1.58	1.53
3	2-A	300[B]	BOG	C4-C5	2.60	1.58	1.53
4	1-A	301[A]	RET	C1-C6	2.72	1.57	1.53
4	1-A	301[A]	RET	C17-C1	2.77	1.59	1.53
4	2-A	301[B]	RET	C1-C6	2.77	1.57	1.53
4	1-A	301[A]	RET	C5-C6	3.33	1.39	1.34
4	2-A	301[B]	RET	C5-C6	3.63	1.40	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2-A	301[B]	RET	C11-C10-C9	-5.47	119.30	127.20
4	1-A	301[A]	RET	C11-C10-C9	-4.46	120.75	127.20
4	1-A	301[A]	RET	C8-C9-C10	-3.74	112.96	118.98
4	2-A	301[B]	RET	C20-C13-C14	-3.33	113.15	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-A	301[A]	RET	C7-C6-C5	-3.17	114.12	121.37
4	1-A	301[A]	RET	C10-C11-C12	-2.95	114.14	123.13
4	2-A	301[B]	RET	C11-C12-C13	-2.77	118.15	126.32
4	2-A	301[B]	RET	C7-C6-C5	-2.68	115.24	121.37
4	2-A	301[B]	RET	C8-C9-C10	-2.68	114.67	118.98
4	2-A	301[B]	RET	C18-C5-C4	-2.52	108.65	113.43
4	1-A	301[A]	RET	C18-C5-C4	-2.32	109.03	113.43
4	2-A	301[B]	RET	C17-C1-C2	-2.06	101.43	108.79
4	2-A	301[B]	RET	C17-C1-C6	2.04	113.50	110.30
4	1-A	301[A]	RET	C19-C9-C8	2.05	121.51	118.10
4	1-A	301[A]	RET	C2-C1-C6	2.09	113.67	110.36
4	1-A	301[A]	RET	C20-C13-C12	2.24	121.83	118.10
4	1-A	301[A]	RET	C17-C1-C6	2.28	113.89	110.30
4	2-A	301[B]	RET	C12-C13-C14	2.29	126.38	118.92
4	2-A	301[B]	RET	C1-C6-C7	2.41	122.58	115.82
4	2-A	301[B]	RET	C2-C1-C6	2.44	114.22	110.36
4	1-A	301[A]	RET	C1-C6-C7	2.71	123.41	115.82
4	1-A	301[A]	RET	C18-C5-C6	6.04	130.54	124.61
4	2-A	301[B]	RET	C18-C5-C6	6.54	131.03	124.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-A	300[A]	BOG	5	0
4	1-A	301[A]	RET	1	0
3	2-A	300[B]	BOG	3	0
4	2-A	301[B]	RET	1	0

## 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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.