



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 09:28 am GMT

PDB ID : 1CVS  
Title : CRYSTAL STRUCTURE OF A DIMERIC FGF2-FGFR1 COMPLEX  
Authors : Plotnikov, A.N.; Schlessinger, J.; Hubbard, S.R.; Mohammadi, M.  
Deposited on : 1999-08-24  
Resolution : 2.80 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

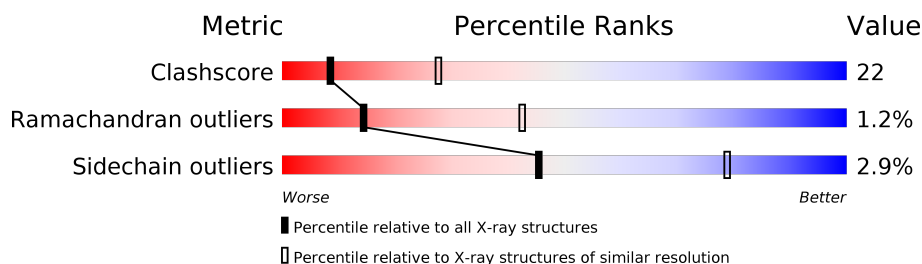
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	122078	3207 (2.80-2.80)
Ramachandran outliers	120005	3156 (2.80-2.80)
Sidechain outliers	119972	3158 (2.80-2.80)

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	A	132	
1	B	132	
2	C	225	
2	D	225	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5173 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 FIBROBLAST GROWTH FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			
1	B	129	Total	C	N	O	S	0	0	0
			1040	660	190	186	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	CYS	ENGINEERED MUTATION	UNP P09038
A	87	SER	CYS	ENGINEERED MUTATION	UNP P09038
B	69	SER	CYS	ENGINEERED MUTATION	UNP P09038
B	87	SER	CYS	ENGINEERED MUTATION	UNP P09038

- Molecule 2 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1588	1015	270	294	9			
2	D	196	Total	C	N	O	S	0	0	0
			1485	951	252	273	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	ASN	ENGINEERED MUTATION	UNP P11362
D	185	GLN	ASN	ENGINEERED MUTATION	UNP P11362

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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



LEU	T331	T332	T333	T334	T335	T336	T337	T338	T339	T340	T341	T342	T343	T344	T345	T346	T347	T348	T349	T350	T351	T352	T353	T354	T355	T356	T357	T358	T359	T360	T361	T362	T363	T364	T365	T366	T367	T368	T369	T370	T371	T372	T373	T374	T375	T376	T377	T378	T379	T380	T381	T382	T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000																																																																																																				
PRO	T231	T232	T233	T234	T235	T236	T237	T238	T239	T240	T241	T242	T243	T244	T245	T246	T247	T248	T249	T250	T251	T252	T253	T254	T255	T256	T257	T258	T259	T260	T261	T262	T263	T264	T265	T266	T267	T268	T269	T270	T271	T272	T273	T274	T275	T276	T277	T278	T279	T280	T281	T282	T283	T284	T285	T286	T287	T288	T289	T290	T291	T292	T293	T294	T295	T296	T297	T298	T299	T300	T301	T302	T303	T304	T305	T306	T307	T308	T309	T310	T311	T312	T313	T314	T315	T316	T317	T318	T319	T320	T321	T322	T323	T324	T325	T326	T327	T328	T329	T330	T331	T332	T333	T334	T335	T336	T337	T338	T339	T340	T341	T342	T343	T344	T345	T346	T347	T348	T349	T350	T351	T352	T353	T354	T355	T356	T357	T358	T359	T360	T361	T362	T363	T364	T365	T366	T367	T368	T369	T370	T371	T372	T373	T374	T375	T376	T377	T378	T379	T380	T381	T382	T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000
ASN	T131	T132	T133	T134	T135	T136	T137	T138	T139	T140	T141	T142	T143	T144	T145	T146	T147	T148	T149	T150	T151	T152	T153	T154	T155	T156	T157	T158	T159	T160	T161	T162	T163	T164	T165	T166	T167	T168	T169	T170	T171	T172	T173	T174	T175	T176	T177	T178	T179	T180	T181	T182	T183	T184	T185	T186	T187	T188	T189	T190	T191	T192	T193	T194	T195	T196	T197	T198	T199	T200	T201	T202	T203	T204	T205	T206	T207	T208	T209	T210	T211	T212	T213	T214	T215	T216	T217	T218	T219	T220	T221	T222	T223	T224	T225	T226	T227	T228	T229	T230	T231	T232	T233	T234																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.45 Å 98.45 Å 197.03 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	96.9 (25.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.240 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5173	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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: 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	0.45	0/1063	0.69	0/1425
1	B	0.46	0/1063	0.69	0/1425
2	C	0.44	0/1635	0.70	0/2244
2	D	0.42	0/1528	0.68	0/2092
All	All	0.44	0/5289	0.69	0/7186

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	280	TYR	Sidechain
2	D	280	TYR	Sidechain



## 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	1040	0	1040	37	0
1	B	1040	0	1040	46	0
2	C	1588	0	1499	68	0
2	D	1485	0	1409	84	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
All	All	5173	0	4988	224	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 22.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LEU:HD12	1:B:124:TYR:HB2	1.59	0.84
2:C:240:ASN:HD22	2:C:240:ASN:C	1.82	0.82
2:C:293:ILE:HD11	2:C:309:GLN:HB2	1.61	0.82
2:D:342:LEU:HD22	2:D:351:HIS:CB	2.13	0.79
1:A:133:GLY:HA3	2:D:200:ASP:HA	1.65	0.78
2:C:260:GLY:O	2:C:261:LEU:HD23	1.83	0.78
1:A:140:LEU:HD13	2:C:169:PRO:HD3	1.66	0.78
2:D:319:THR:HG22	2:D:321:LYS:H	1.50	0.76
2:D:185:GLN:HA	2:D:185:GLN:NE2	2.03	0.73
2:D:190:TRP:CZ3	2:D:230:CYS:HB3	2.23	0.73
2:D:203:ILE:N	2:D:203:ILE:HD13	2.04	0.73
2:D:342:LEU:HD22	2:D:351:HIS:HB3	1.72	0.70
2:C:172:LYS:O	2:C:220:VAL:HG22	1.92	0.70
2:D:203:ILE:H	2:D:203:ILE:HD13	1.56	0.69
2:C:282:ASP:HB3	2:C:283:PRO:CD	2.22	0.68
2:C:233:GLU:HG3	2:C:238:SER:HB3	1.76	0.68
2:C:314:ALA:HB2	2:C:323:MET:HG3	1.75	0.68
2:D:262:PRO:HG2	2:D:354:ALA:HB2	1.75	0.68
2:D:203:ILE:H	2:D:203:ILE:CD1	2.07	0.67
2:D:282:ASP:HB3	2:D:283:PRO:CD	2.26	0.66
2:D:161:MET:HE1	2:D:178:CYS:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH1	1:B:43:VAL:HG11	2.13	0.64
2:D:292:HIS:HD2	2:D:338:GLU:HG2	1.64	0.63
2:D:342:LEU:HD22	2:D:351:HIS:HB2	1.80	0.63
2:C:256:ILE:HD12	2:C:256:ILE:N	2.13	0.63
2:C:253:HIS:CE1	2:C:256:ILE:HD11	2.35	0.62
1:A:72:ARG:HD3	1:A:84:ALA:O	1.99	0.62
1:A:24:TYR:OH	2:C:163:LYS:HE3	2.00	0.62
2:D:257:LEU:CD2	2:D:279:VAL:HG22	2.30	0.61
1:B:98:LEU:HD13	2:D:250:ARG:CZ	2.30	0.61
1:B:131:GLY:N	1:B:134:GLN:NE2	2.48	0.61
1:A:118:LEU:HD23	1:A:124:TYR:HA	1.80	0.61
2:D:225:LYS:HE2	2:D:247:VAL:O	2.00	0.61
1:B:76:MET:HE1	1:B:114:TRP:HB2	1.82	0.61
2:C:240:ASN:ND2	2:C:240:ASN:C	2.54	0.61
1:B:76:MET:CE	1:B:114:TRP:HB2	2.30	0.61
1:B:59:GLU:HA	2:D:286:HIS:ND1	2.16	0.60
2:D:271:SER:O	2:D:330:ASN:HA	2.01	0.60
2:C:340:THR:HG22	2:C:342:LEU:HD12	1.83	0.60
2:D:185:GLN:HA	2:D:185:GLN:HE21	1.67	0.60
1:B:55:LEU:CD1	1:B:65:ILE:HG12	2.31	0.60
2:D:358:VAL:O	2:D:359:LEU:HD23	2.02	0.59
2:C:192:LYS:HE2	2:C:228:TYR:OH	2.03	0.59
2:D:319:THR:HG22	2:D:321:LYS:HG3	1.83	0.59
1:B:138:LEU:HD11	2:C:204:GLY:HA2	1.84	0.59
2:C:153:PRO:HA	2:C:181:SER:O	2.03	0.59
2:D:199:PRO:HA	2:D:206:TYR:CE1	2.38	0.59
2:C:170:ALA:O	2:C:171:ALA:HB3	2.02	0.59
2:C:199:PRO:HA	2:C:206:TYR:CE1	2.39	0.58
2:D:319:THR:HG21	2:D:321:LYS:HE3	1.84	0.58
2:D:170:ALA:O	2:D:171:ALA:HB3	2.03	0.58
2:C:257:LEU:HD13	2:C:277:CYS:SG	2.44	0.58
2:D:319:THR:CG2	2:D:321:LYS:HG3	2.34	0.57
1:B:79:ASP:CG	1:B:81:ARG:HH11	2.07	0.57
2:C:273:VAL:HG13	2:C:328:LEU:HB2	1.86	0.57
2:C:319:THR:HG22	2:C:321:LYS:HG3	1.86	0.57
2:C:265:LYS:HB2	2:C:356:LEU:HD23	1.87	0.57
1:B:96:GLU:HG3	1:B:106:TYR:CE1	2.40	0.57
1:A:83:LEU:C	1:A:83:LEU:HD12	2.26	0.56
2:C:338:GLU:HB2	2:C:355:TRP:CZ3	2.40	0.56
2:D:251:SER:HB2	2:D:282:ASP:HB2	1.88	0.56
2:C:197:PHE:O	2:C:206:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:257:LEU:HB2	2:C:352:HIS:CE1	2.40	0.56
2:D:312:LYS:HG2	2:D:323:MET:SD	2.46	0.56
1:A:78:GLU:HA	1:A:111:TYR:CZ	2.41	0.56
2:C:180:SER:OG	2:C:232:VAL:HG11	2.06	0.56
2:D:203:ILE:N	2:D:203:ILE:CD1	2.68	0.56
2:D:163:LYS:HE2	2:D:166:HIS:CD2	2.40	0.55
2:D:282:ASP:HB3	2:D:283:PRO:HD3	1.87	0.55
1:A:71:ASN:O	1:A:71:ASN:ND2	2.40	0.55
2:C:303:ASP:OD2	2:C:305:LEU:HB2	2.07	0.55
2:D:153:PRO:HA	2:D:181:SER:O	2.07	0.55
2:D:340:THR:HG22	2:D:342:LEU:HD23	1.88	0.55
2:D:185:GLN:CA	2:D:185:GLN:HE21	2.18	0.55
2:D:292:HIS:CD2	2:D:338:GLU:HG2	2.41	0.54
1:B:98:LEU:HD13	2:D:250:ARG:NH2	2.22	0.54
2:D:189:ARG:HG3	2:D:231:ILE:HB	1.90	0.54
2:D:161:MET:CE	2:D:178:CYS:HA	2.37	0.54
1:A:134:GLN:O	1:A:137:ILE:HG12	2.07	0.54
1:B:23:LEU:HG	1:B:53:LEU:HD12	1.90	0.54
2:D:314:ALA:HB2	2:D:323:MET:HG3	1.88	0.54
1:A:78:GLU:HA	1:A:111:TYR:CE1	2.42	0.54
1:B:55:LEU:N	1:B:55:LEU:HD22	2.22	0.53
2:D:165:LEU:HD12	2:D:166:HIS:N	2.22	0.53
2:D:279:VAL:HG12	2:D:280:TYR:N	2.22	0.53
1:B:76:MET:HE2	1:B:108:SER:HB2	1.90	0.53
2:C:255:PRO:C	2:C:256:ILE:HD12	2.28	0.52
2:C:282:ASP:HB3	2:C:283:PRO:HD3	1.92	0.52
2:D:342:LEU:CD2	2:D:351:HIS:HB2	2.39	0.52
1:A:101:ASN:O	1:A:102:ASN:HB2	2.10	0.52
1:A:104:ASN:OD1	2:C:250:ARG:NH2	2.37	0.52
1:A:33:ARG:CZ	1:A:43:VAL:HG11	2.40	0.51
1:B:101:ASN:O	1:B:102:ASN:HB2	2.09	0.51
2:C:150:PRO:HB3	2:C:236:TYR:CZ	2.45	0.51
1:B:76:MET:HE1	1:B:114:TRP:CB	2.40	0.51
1:B:59:GLU:HA	2:D:286:HIS:CE1	2.46	0.51
2:C:149:MET:HG3	2:C:149:MET:O	2.11	0.51
2:C:166:HIS:CG	2:C:176:PHE:HE1	2.29	0.51
2:C:319:THR:CG2	2:C:321:LYS:HG3	2.42	0.50
2:D:325:VAL:O	2:D:325:VAL:HG13	2.11	0.50
1:B:79:ASP:OD2	1:B:81:ARG:HG2	2.12	0.50
1:B:107:ARG:HD2	1:B:112:THR:O	2.13	0.49
2:C:319:THR:HG21	2:C:321:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:THR:HG22	2:D:323:MET:SD	2.52	0.49
2:C:155:TRP:CE2	2:C:239:ILE:HD12	2.48	0.49
2:C:293:ILE:CD1	2:C:309:GLN:HB2	2.38	0.49
2:C:338:GLU:HB2	2:C:355:TRP:CE3	2.47	0.49
1:A:90:ASP:OD2	1:A:110:LYS:HD2	2.12	0.49
2:C:358:VAL:O	2:C:359:LEU:HD23	2.13	0.49
2:C:290:LEU:HD23	2:C:308:VAL:HG11	1.95	0.49
2:D:197:PHE:O	2:D:206:TYR:OH	2.23	0.49
2:C:262:PRO:HG2	2:C:354:ALA:HB2	1.95	0.48
2:C:296:ASN:OD1	2:C:296:ASN:N	2.45	0.48
2:C:261:LEU:HA	2:C:262:PRO:C	2.33	0.48
1:A:58:GLU:HG2	1:A:93:PHE:CE1	2.49	0.48
1:A:33:ARG:CZ	1:A:43:VAL:CG1	2.92	0.48
1:A:36:PRO:HA	1:A:70:ALA:CB	2.44	0.48
1:B:48:ASP:HB3	1:B:51:ILE:HG23	1.96	0.48
1:B:120:ARG:HG3	3:B:2:SO4:O2	2.14	0.47
1:A:55:LEU:CD2	1:A:55:LEU:N	2.77	0.47
2:C:198:LYS:H	2:C:201:HIS:CE1	2.32	0.47
2:D:170:ALA:O	2:D:171:ALA:CB	2.63	0.47
2:C:234:ASN:C	2:C:234:ASN:OD1	2.53	0.47
2:C:257:LEU:HD12	2:C:352:HIS:HB2	1.97	0.47
1:A:65:ILE:HD12	1:A:74:LEU:HD23	1.97	0.47
2:C:271:SER:O	2:C:330:ASN:HA	2.15	0.47
1:A:81:ARG:HB2	1:A:124:TYR:OH	2.16	0.46
1:B:37:ASP:OD1	1:B:37:ASP:C	2.54	0.46
2:D:269:LEU:HD23	2:D:270:GLY:N	2.31	0.46
1:B:131:GLY:H	1:B:134:GLN:NE2	2.13	0.46
2:C:253:HIS:CE1	2:C:256:ILE:CD1	2.98	0.46
2:D:178:CYS:N	2:D:179:PRO:HD3	2.31	0.46
2:D:155:TRP:CZ3	2:D:178:CYS:HB3	2.50	0.46
2:D:189:ARG:CG	2:D:231:ILE:HB	2.45	0.46
2:D:273:VAL:HG13	2:D:328:LEU:HB2	1.97	0.46
2:D:291:LYS:HB2	2:D:311:LEU:HD11	1.96	0.46
1:B:82:LEU:HD12	1:B:124:TYR:CB	2.37	0.46
2:D:255:PRO:HD3	2:D:345:ASN:ND2	2.31	0.46
2:D:212:THR:HG22	2:D:212:THR:O	2.16	0.46
1:A:97:ARG:HD3	1:A:99:GLU:OE1	2.16	0.45
1:B:36:PRO:HA	1:B:70:ALA:CB	2.46	0.45
2:C:233:GLU:HG3	2:C:238:SER:CB	2.45	0.45
2:D:287:ILE:HG22	2:D:288:GLN:N	2.30	0.45
2:D:356:LEU:HD23	2:D:357:THR:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:HIS:CE1	1:B:18:LYS:CB	3.00	0.45
2:C:170:ALA:O	2:C:171:ALA:CB	2.64	0.45
2:D:272:ASN:OD1	2:D:329:ARG:HA	2.17	0.45
2:C:233:GLU:CG	2:C:238:SER:HB3	2.46	0.45
2:D:184:PRO:HD2	2:D:236:TYR:HE1	1.81	0.45
2:D:265:LYS:HG2	2:D:275:PHE:CE1	2.51	0.45
1:B:48:ASP:OD2	1:B:49:PRO:HD2	2.16	0.45
2:D:318:THR:HG23	2:D:322:GLU:HG3	1.97	0.45
1:B:24:TYR:CZ	1:B:29:GLY:HA2	2.52	0.45
1:B:76:MET:O	1:B:91:GLU:HB3	2.17	0.45
1:A:115:TYR:HB2	1:A:137:ILE:HG22	1.99	0.45
2:C:319:THR:HG22	2:C:321:LYS:H	1.82	0.44
1:B:59:GLU:HA	2:D:286:HIS:CG	2.52	0.44
2:C:334:GLU:HG3	2:C:334:GLU:H	1.52	0.44
2:D:163:LYS:HE2	2:D:166:HIS:CG	2.52	0.44
2:D:190:TRP:CH2	2:D:230:CYS:HB3	2.53	0.44
2:D:318:THR:CG2	2:D:323:MET:SD	3.05	0.44
2:C:279:VAL:HG12	2:C:280:TYR:N	2.31	0.44
2:D:163:LYS:HG2	2:D:163:LYS:O	2.17	0.44
2:D:281:SER:HB3	2:D:285:PRO:HD3	2.00	0.44
1:B:81:ARG:HB2	1:B:124:TYR:OH	2.16	0.44
2:D:187:THR:O	2:D:232:VAL:HA	2.18	0.44
1:A:33:ARG:NH1	1:A:43:VAL:HG11	2.33	0.44
1:A:55:LEU:HD22	1:A:55:LEU:N	2.33	0.43
2:C:187:THR:O	2:C:232:VAL:HA	2.18	0.43
1:B:48:ASP:CG	1:B:49:PRO:HD2	2.38	0.43
2:D:183:THR:HA	2:D:184:PRO:C	2.37	0.43
1:B:35:HIS:HE2	1:B:41:ASP:CG	2.20	0.43
2:D:234:ASN:OD1	2:D:234:ASN:C	2.57	0.43
2:D:327:HIS:O	2:D:328:LEU:HD23	2.19	0.43
1:A:120:ARG:HG3	3:A:3:SO4:O2	2.19	0.43
2:C:188:LEU:HD12	2:C:213:TRP:HA	2.00	0.43
2:D:288:GLN:HG3	2:D:312:LYS:O	2.18	0.43
1:A:55:LEU:HD13	1:A:65:ILE:HG12	2.00	0.43
1:B:22:ARG:HH12	1:B:52:LYS:HE2	1.84	0.43
1:B:99:GLU:HB2	1:B:101:ASN:OD1	2.19	0.43
1:B:72:ARG:HB3	1:B:84:ALA:HB1	2.00	0.43
2:D:156:THR:HG23	2:D:180:SER:C	2.38	0.43
1:A:23:LEU:HG	1:A:53:LEU:HD12	2.01	0.43
2:D:175:LYS:HA	2:D:215:ILE:O	2.19	0.43
1:B:83:LEU:C	1:B:83:LEU:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:THR:HA	2:C:184:PRO:C	2.38	0.42
1:B:78:GLU:HA	1:B:111:TYR:CZ	2.55	0.42
2:C:314:ALA:CB	2:C:323:MET:HG3	2.48	0.42
1:A:95:PHE:HD1	1:A:107:ARG:CZ	2.33	0.42
1:B:36:PRO:HA	1:B:70:ALA:HB1	2.02	0.42
2:D:257:LEU:HB2	2:D:352:HIS:CE1	2.54	0.42
1:A:36:PRO:HA	1:A:70:ALA:HB1	2.00	0.42
2:C:282:ASP:HB3	2:C:283:PRO:HD2	2.02	0.42
1:B:49:PRO:HG2	1:B:50:HIS:CD2	2.54	0.42
2:C:269:LEU:HD12	2:C:333:PHE:CD2	2.55	0.42
2:C:250:ARG:HB3	2:C:282:ASP:OD1	2.20	0.42
2:D:279:VAL:CG1	2:D:280:TYR:N	2.83	0.42
2:C:341:CYS:O	2:C:351:HIS:HA	2.20	0.42
1:A:16:HIS:CE1	1:A:18:LYS:CB	3.03	0.41
1:B:97:ARG:HD3	1:B:99:GLU:OE1	2.20	0.41
1:A:37:ASP:OD2	1:A:39:ARG:NE	2.53	0.41
2:C:273:VAL:HG22	2:C:274:GLU:N	2.35	0.41
1:A:24:TYR:CZ	1:A:29:GLY:HA2	2.55	0.41
2:C:155:TRP:CD2	2:C:239:ILE:HD12	2.55	0.41
2:D:257:LEU:HD23	2:D:279:VAL:HG22	2.01	0.41
1:A:56:GLN:O	1:A:63:VAL:HA	2.21	0.41
1:A:77:LYS:HG2	1:A:81:ARG:O	2.21	0.41
1:B:124:TYR:C	1:B:124:TYR:CD1	2.94	0.41
2:D:188:LEU:HD22	2:D:189:ARG:N	2.36	0.41
2:D:189:ARG:HE	2:D:231:ILE:HG21	1.86	0.41
1:A:76:MET:HE3	1:A:114:TRP:HB2	2.02	0.41
1:B:129:LYS:HE3	1:B:129:LYS:HB2	1.91	0.41
2:C:292:HIS:CD2	2:C:338:GLU:HG2	2.55	0.41
2:D:155:TRP:HZ3	2:D:178:CYS:HB3	1.86	0.41
1:A:131:GLY:O	1:A:137:ILE:HD13	2.21	0.41
1:B:55:LEU:HD12	1:B:65:ILE:HG12	1.99	0.41
2:C:186:PRO:HB2	2:C:232:VAL:HG12	2.03	0.41
2:C:252:PRO:C	2:C:347:ILE:HD13	2.41	0.41
2:D:254:ARG:HG2	2:D:254:ARG:HH11	1.84	0.41
1:B:118:LEU:HD23	1:B:124:TYR:HA	2.02	0.41
2:C:149:MET:O	2:C:151:VAL:HG23	2.21	0.41
2:D:253:HIS:CE1	2:D:256:ILE:HD13	2.55	0.40
2:D:166:HIS:O	2:D:245:LEU:HD12	2.22	0.40
1:A:133:GLY:HA2	2:D:202:ARG:O	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	127/132 (96%)	121 (95%)	5 (4%)	1 (1%)	21	53
1	B	127/132 (96%)	121 (95%)	5 (4%)	1 (1%)	21	53
2	C	209/225 (93%)	195 (93%)	10 (5%)	4 (2%)	9	28
2	D	192/225 (85%)	183 (95%)	7 (4%)	2 (1%)	17	48
All	All	655/714 (92%)	620 (95%)	27 (4%)	8 (1%)	14	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	B	112	THR
2	C	330	ASN
2	D	330	ASN
2	C	296	ASN
2	D	219	SER
2	C	219	SER
2	C	251	SER

### 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	110/113 (97%)	108 (98%)	2 (2%)	62	88
1	B	110/113 (97%)	109 (99%)	1 (1%)	81	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	168/198 (85%)	161 (96%)	7 (4%)	32	66
2	D	158/198 (80%)	152 (96%)	6 (4%)	36	70
All	All	546/622 (88%)	530 (97%)	16 (3%)	45	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	128	SER
1	B	55	LEU
2	C	188	LEU
2	C	212	THR
2	C	240	ASN
2	C	318	THR
2	C	322	GLU
2	C	334	GLU
2	C	356	LEU
2	D	188	LEU
2	D	203	ILE
2	D	239	ILE
2	D	278	LYS
2	D	355	TRP
2	D	356	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	185	GLN
2	C	240	ASN
2	C	241	HIS
2	C	288	GLN
2	C	317	ASN
2	D	166	HIS
2	D	185	GLN
2	D	241	HIS
2	D	284	GLN
2	D	317	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	SO4	A	3	-	4,4,4	0.32	0	6,6,6	0.11	0
3	SO4	A	4	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	B	1	-	4,4,4	0.34	0	6,6,6	0.06	0
3	SO4	B	2	-	4,4,4	0.36	0	6,6,6	0.11	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	SO4	A	3	-	-	0/0/0/0	0/0/0/0
3	SO4	A	4	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	SO4	1	0
3	B	2	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.