



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:04 PM GMT

PDB ID : 4BE7
Title : MUTANT (K220R) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP
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Deposited on : 2013-03-06
Resolution : 2.74 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

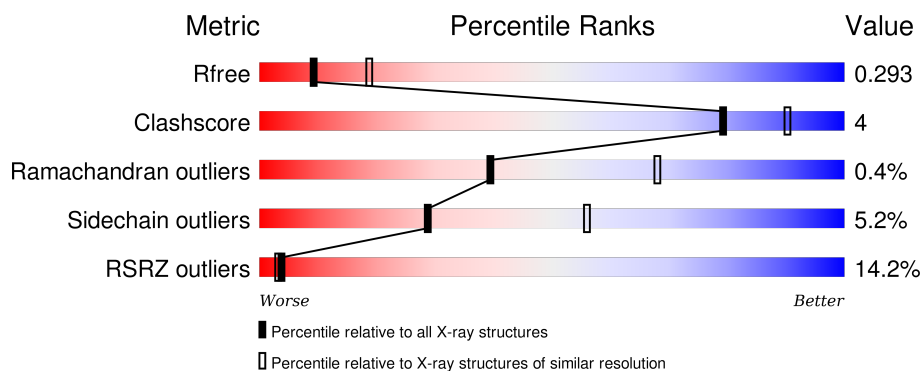
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	1038	
1	D	1038	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13387 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.

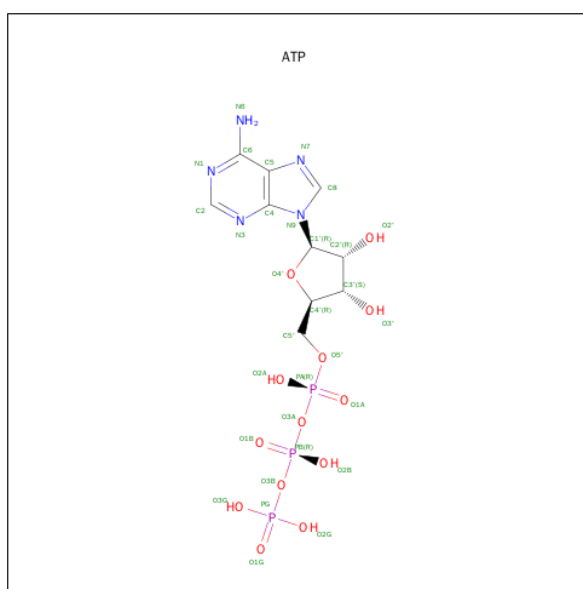
- Molecule 1 is a protein called TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	837	Total	C	N	O	S	0	0	0
			6631	4226	1112	1277	16			
1	D	835	Total	C	N	O	S	0	0	0
			6594	4204	1106	1268	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	220	ARG	LYS	ENGINEERED MUTATION	UNP Q304R3
D	220	ARG	LYS	ENGINEERED MUTATION	UNP Q304R3

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

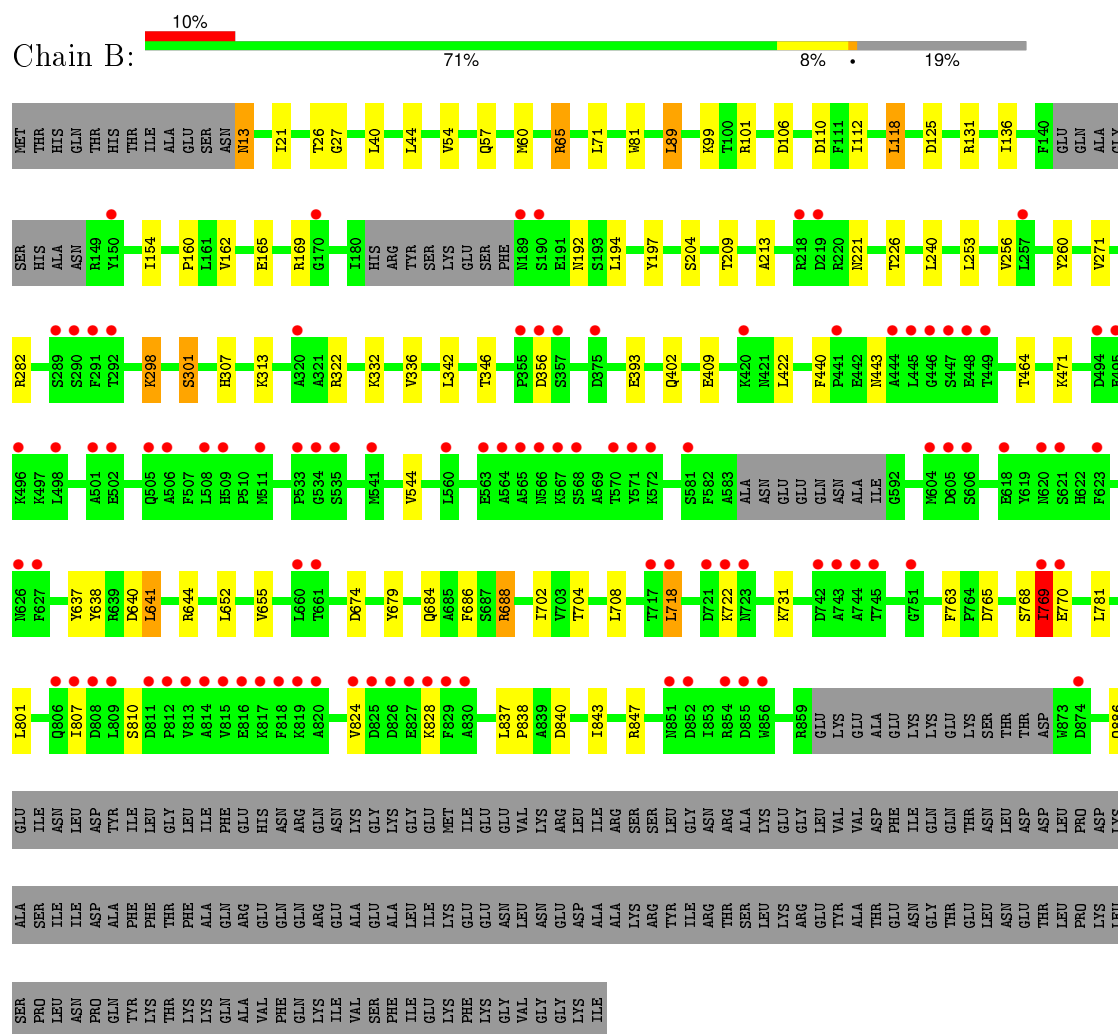
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	45	Total 45	O 45	0	0
5	D	33	Total 33	O 33	0	0

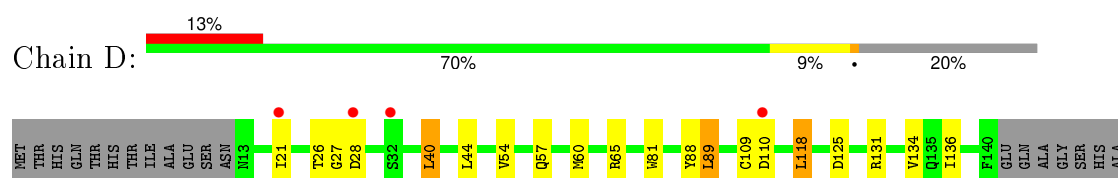
3 Residue-property plots

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

• Molecule 1: TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN



• Molecule 1: TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN



LYS	ILE	VAL	SER	PHE	ILE	GLU	LYS	GLN	ARG
E821	E822	E823	V824	D825	E827	K828	L832	L837	L838
E829	E830	E831	E832	E833	E834	E835	E836	E837	E838
E839	E840	E841	E842	E843	E844	E845	E846	E847	E848
E849	E850	E851	E852	E853	E854	E855	E856	E857	E858
E859	E860	E861	E862	E863	E864	E865	E866	E867	E868
E869	E870	E871	E872	E873	E874	E875	E876	E877	E878
E879	E880	E881	E882	E883	E884	E885	E886	E887	E888
E889	E890	E891	E892	E893	E894	E895	E896	E897	E898
E899	E900	E901	E902	E903	E904	E905	E906	E907	E908
E909	E910	E911	E912	E913	E914	E915	E916	E917	E918
E919	E920	E921	E922	E923	E924	E925	E926	E927	E928
E929	E930	E931	E932	E933	E934	E935	E936	E937	E938
E939	E940	E941	E942	E943	E944	E945	E946	E947	E948
E949	E950	E951	E952	E953	E954	E955	E956	E957	E958
E959	E960	E961	E962	E963	E964	E965	E966	E967	E968
E969	E970	E971	E972	E973	E974	E975	E976	E977	E978
E979	E980	E981	E982	E983	E984	E985	E986	E987	E988
E989	E990	E991	E992	E993	E994	E995	E996	E997	E998
E999	F000	F001	F002	F003	F004	F005	F006	F007	F008
F009	F010	F011	F012	F013	F014	F015	F016	F017	F018
F019	F020	F021	F022	F023	F024	F025	F026	F027	F028
F029	F030	F031	F032	F033	F034	F035	F036	F037	F038
F039	F040	F041	F042	F043	F044	F045	F046	F047	F048
F049	F050	F051	F052	F053	F054	F055	F056	F057	F058
F059	F060	F061	F062	F063	F064	F065	F066	F067	F068
F069	F070	F071	F072	F073	F074	F075	F076	F077	F078
F079	F080	F081	F082	F083	F084	F085	F086	F087	F088
F089	F090	F091	F092	F093	F094	F095	F096	F097	F098
F099	F100	F101	F102	F103	F104	F105	F106	F107	F108
F109	F110	F111	F112	F113	F114	F115	F116	F117	F118
F119	F120	F121	F122	F123	F124	F125	F126	F127	F128
F129	F130	F131	F132	F133	F134	F135	F136	F137	F138
F139	F140	F141	F142	F143	F144	F145	F146	F147	F148
F149	F150	F151	F152	F153	F154	F155	F156	F157	F158
F159	F160	F161	F162	F163	F164	F165	F166	F167	F168
F169	F170	F171	F172	F173	F174	F175	F176	F177	F178
F179	F180	F181	F182	F183	F184	F185	F186	F187	F188
F189	F190	F191	F192	F193	F194	F195	F196	F197	F198
F199	F200	F201	F202	F203	F204	F205	F206	F207	F208
F209	F210	F211	F212	F213	F214	F215	F216	F217	F218
F219	F220	F221	F222	F223	F224	F225	F226	F227	F228
F229	F230	F231	F232	F233	F234	F235	F236	F237	F238
F239	F240	F241	F242	F243	F244	F245	F246	F247	F248
F249	F250	F251	F252	F253	F254	F255	F256	F257	F258
F259	F260	F261	F262	F263	F264	F265	F266	F267	F268
F269	F270	F271	F272	F273	F274	F275	F276	F277	F278
F279	F280	F281	F282	F283	F284	F285	F286	F287	F288
F289	F290	F291	F292	F293	F294	F295	F296	F297	F298
F299	F300	F301	F302	F303	F304	F305	F306	F307	F308
F309	F310	F311	F312	F313	F314	F315	F316	F317	F318
F319	F320	F321	F322	F323	F324	F325	F326	F327	F328
F329	F330	F331	F332	F333	F334	F335	F336	F337	F338
F339	F340	F341	F342	F343	F344	F345	F346	F347	F348
F349	F350	F351	F352	F353	F354	F355	F356	F357	F358
F359	F360	F361	F362	F363	F364	F365	F366	F367	F368
F369	F370	F371	F372	F373	F374	F375	F376	F377	F378
F379	F380	F381	F382	F383	F384	F385	F386	F387	F388
F389	F390	F391	F392	F393	F394	F395	F396	F397	F398
F399	F400	F401	F402	F403	F404	F405	F406	F407	F408
F409	F410	F411	F412	F413	F414	F415	F416	F417	F418
F419	F420	F421	F422	F423	F424	F425	F426	F427	F428
F429	F430	F431	F432	F433	F434	F435	F436	F437	F438
F439	F440	F441	F442	F443	F444	F445	F446	F447	F448
F449	F450	F451	F452	F453	F454	F455	F456	F457	F458
F459	F460	F461	F462	F463	F464	F465	F466	F467	F468
F469	F470	F471	F472	F473	F474	F475	F476	F477	F478
F479	F480	F481	F482	F483	F484	F485	F486	F487	F488
F489	F490	F491	F492	F493	F494	F495	F496	F497	F498
F499	F500	F501	F502	F503	F504	F505	F506	F507	F508
F509	F510	F511	F512	F513	F514	F515	F516	F517	F518
F519	F520	F521	F522	F523	F524	F525	F526	F527	F528
F529	F530	F531	F532	F533	F534	F535	F536	F537	F538
F539	F540	F541	F542	F543	F544	F545	F546	F547	F548
F549	F550	F551	F552	F553	F554	F555	F556	F557	F558
F559	F560	F561	F562	F563	F564	F565	F566	F567	F568
F569	F570	F571	F572	F573	F574	F575	F576	F577	F578
F579	F580	F581	F582	F583	F584	F585	F586	F587	F588
F589	F590	F591	F592	F593	F594	F595	F596	F597	F598
F599	F600	F601	F602	F603	F604	F605	F606	F607	F608
F609	F610	F611	F612	F613	F614	F615	F616	F617	F618
F619	F620	F621	F622	F623	F624	F625	F626	F627	F628
F629	F630	F631	F632	F633	F634	F635	F636	F637	F638
F639	F640	F641	F642	F643	F644	F645	F646	F647	F648
F649	F650	F651	F652	F653	F654	F655	F656	F657	F658
F659	F660	F661	F662	F663	F664	F665	F666	F667	F668
F669	F670	F671	F672	F673	F674	F675	F676	F677	F678
F679	F680	F681	F682	F683	F684	F685	F686	F687	F688
F689	F690	F691	F692	F693	F694	F695	F696	F697	F698
F699	F700	F701	F702	F703	F704	F705	F706	F707	F708
F709	F710	F711	F712	F713	F714	F715	F716	F717	F718
F719	F720	F721	F722	F723	F724	F725	F726	F727	F728
F729	F730	F731	F732	F733	F734	F735	F736	F737	F738
F739	F740	F741	F742	F743	F744	F745	F746	F747	F748
F749	F750	F751	F752	F753	F754	F755	F756	F757	F758
F759	F760	F761	F762	F763	F764	F765	F766	F767	F768
F769	F770	F771	F772	F773	F774	F775	F776	F777	F778
F779	F780	F781	F782	F783	F784	F785	F786	F787	F788
F789	F790	F791	F792	F793	F794	F795	F796	F797	F798
F799	F800	F801	F802	F803	F804	F805	F806	F807	F808
F809	F810	F811	F812	F813	F814	F815	F816	F817	F818
F819	F820	F821	F822	F823	F824	F825	F826	F827	F828
F829	F830	F831	F832	F833	F834	F835	F836	F837	F838
F839	F840	F841	F842	F843	F844	F845	F846	F847	F848
F849	F850	F851	F852	F853	F854	F855	F856	F857	F858
F859	F860	F861	F862	F863	F864	F865	F866	F867	F868
F869	F870	F871	F872	F873	F874	F875	F876	F877	F878
F879	F880	F881	F882	F883	F884	F885	F886	F887	F888
F889	F890	F891	F892	F893	F894	F895	F896	F897	F898
F899	F900	F901	F902	F903	F904	F905	F906	F907	F908
F909	F910	F911	F912	F913	F914	F915	F916	F917	F918
F919	F920	F921	F922	F923	F924	F925	F926	F927	F928
F929	F930	F931	F932	F933	F934	F935	F936	F937	F938
F939	F940	F941	F942	F943	F944	F945	F946	F947	F948
F949	F950	F951	F952	F953	F954	F955	F956	F957	F958
F959	F960	F961	F962	F963	F964	F965	F966	F967	F968
F969	F970	F971	F972	F973	F974	F975	F976	F977	F978
F979	F980	F981	F982	F983	F984	F985	F986	F987	F988
F989	F990	F991	F992	F993	F994	F995	F996	F997	F998
F999	G000	G001	G002	G003	G004	G005	G006	G007	G008
G009	G010	G011	G012	G013	G014	G015	G016	G017	G018
G019	G020	G021	G022	G023	G024	G025	G026	G027	G028
G029	G030	G031	G032	G033	G034	G035	G036	G037	G038
G039	G040	G041	G042	G043	G044	G045	G046	G047	G048
G049	G050	G051	G052	G053	G054	G055	G056	G057	G058
G059	G060	G061	G062	G063	G064	G065	G066	G067	G068
G069	G070	G071	G072	G073	G074	G075	G076	G077	G078
G079	G080	G081	G082	G083	G084	G085	G086	G087	G088
G089	G090	G091	G092	G093	G094	G095	G096	G097	G098
G099	G100	G101	G102	G103	G104	G105	G106	G107	G108
G109	G110	G111	G112	G113	G114	G115	G116	G117	G118
G119	G120	G121	G122	G123	G124	G125	G126	G127	G128
G129	G130	G131	G132	G133	G134	G135	G136	G137	G138
G139	G140	G141	G142	G143	G144	G145	G146	G147	G148
G149	G150	G151	G152	G153	G154	G155	G156	G157	G158
G159	G160	G161	G162	G163	G164	G165	G166	G167	G168
G169	G170	G171	G172	G173	G174	G175	G176	G177	G178
G179	G180	G181	G182	G183	G184	G185	G186	G187	G188
G189	G190	G191	G192	G193	G194	G195	G196	G197	G198
G199	G200	G201	G202	G203	G204	G205	G206	G207	G208
G209	G210	G211	G212	G213	G214	G215	G216	G217	G218
G219	G220	G221	G222	G223	G224	G225	G226	G227	G228
G229	G230	G231	G232	G233	G234	G235			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.05Å 124.35Å 128.01Å 90.00° 108.86° 90.00°	Depositor
Resolution (Å)	32.36 – 2.74 33.73 – 2.74	Depositor EDS
% Data completeness (in resolution range)	93.2 (32.36-2.74) 93.5 (33.73-2.74)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.249 , 0.292 0.249 , 0.293	Depositor DCC
R_{free} test set	3192 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.6	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63146 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13387	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, PO4, ATP

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	B	0.27	0/6760	0.52	1/9146 (0.0%)
1	D	0.27	0/6721	0.53	3/9097 (0.0%)
All	All	0.27	0/13481	0.53	4/18243 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	441	PRO	C-N-CA	6.15	137.08	121.70
1	D	441	PRO	CA-C-N	5.29	128.83	117.20
1	B	769	ILE	N-CA-C	-5.26	96.79	111.00
1	D	826	ASP	C-N-CA	5.03	134.27	121.70

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	B	6631	0	6305	44	0
1	D	6594	0	6268	47	0
2	B	31	0	12	1	0
2	D	31	0	12	1	0
3	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	45	0	0	1	0
5	D	33	0	0	1	0
All	All	13387	0	12597	91	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 4.

All (91) 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:D:824:VAL:HG13	1:D:828:LYS:HB3	1.54	0.90
1:D:27:GLY:HA2	1:D:28:ASP:HB2	1.59	0.85
1:D:169:ARG:HG3	1:D:169:ARG:HH11	1.52	0.73
1:D:465:ASP:OD1	1:D:468:ARG:NH2	2.22	0.71
1:D:322:ARG:NH2	5:D:2021:HOH:O	2.25	0.69
1:B:770:GLU:N	1:B:770:GLU:OE1	2.25	0.68
1:D:440:PHE:O	1:D:443:ASN:ND2	2.28	0.66
1:D:801:LEU:HG	1:D:837:LEU:HD11	1.78	0.65
1:B:322:ARG:NH2	5:B:2025:HOH:O	2.29	0.65
1:B:769:ILE:HG22	1:B:770:GLU:HA	1.79	0.65
1:B:213:ALA:HB2	1:B:271:VAL:HG23	1.81	0.63
1:D:440:PHE:N	1:D:443:ASN:OD1	2.29	0.62
1:D:54:VAL:HG11	1:D:60:MET:HG3	1.82	0.62
1:B:226:THR:O	1:B:471:LYS:NZ	2.30	0.62
1:D:684:GLN:O	1:D:688:ARG:NH1	2.32	0.62
1:D:213:ALA:HB2	1:D:271:VAL:HG23	1.82	0.62
1:D:688:ARG:NH2	2:D:1887:ATP:O1G	2.30	0.61
1:B:154:ILE:HB	1:B:162:VAL:HB	1.81	0.60
1:D:154:ILE:HB	1:D:162:VAL:HB	1.83	0.60
1:D:678:ARG:NH1	1:D:711:SER:OG	2.34	0.60
1:B:298:LYS:O	1:B:301:SER:OG	2.21	0.58
1:B:65:ARG:HG3	1:B:81:TRP:CD2	2.39	0.58
1:B:110:ASP:HB2	1:B:118:LEU:HD21	1.86	0.57
1:B:313:LYS:NZ	1:B:409:GLU:OE1	2.32	0.57
1:B:443:ASN:HB3	1:B:718:LEU:HD11	1.86	0.57
1:D:309:THR:HA	1:D:313:LYS:HE2	1.86	0.56
1:B:89:LEU:O	1:B:99:LYS:NZ	2.38	0.56
1:B:13:ASN:HD22	1:B:13:ASN:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:LYS:NZ	1:D:409:GLU:OE1	2.37	0.55
1:D:54:VAL:HG11	1:D:60:MET:CG	2.37	0.55
1:B:44:LEU:HD13	1:B:136:ILE:HG21	1.89	0.54
1:B:54:VAL:HG11	1:B:60:MET:HG3	1.90	0.53
1:B:688:ARG:NH2	2:B:1887:ATP:O1G	2.34	0.53
1:B:824:VAL:HG13	1:B:828:LYS:HB3	1.89	0.53
1:B:838:PRO:HG2	1:B:843:ILE:HD11	1.92	0.52
1:D:189:ASN:HA	1:D:192:ASN:OD1	2.10	0.51
1:B:801:LEU:HG	1:B:837:LEU:HD11	1.91	0.51
1:B:54:VAL:HG11	1:B:60:MET:CG	2.41	0.51
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.38	0.51
1:B:204:SER:HB2	1:B:209:THR:HG23	1.94	0.50
1:D:325:THR:HG21	1:D:378:ILE:HB	1.94	0.50
1:D:88:TYR:CE1	1:D:109:CYS:HB2	2.47	0.49
1:D:125:ASP:OD2	1:D:131:ARG:NH1	2.45	0.49
1:B:686:PHE:CZ	1:B:702:ILE:HG21	2.49	0.48
1:D:110:ASP:HB2	1:D:118:LEU:HD21	1.95	0.48
1:B:26:THR:OG1	1:B:27:GLY:HA2	2.13	0.48
1:D:679:TYR:CD1	1:D:718:LEU:HD12	2.49	0.48
1:B:256:VAL:HA	1:B:260:TYR:HB2	1.94	0.47
1:D:581:SER:O	1:D:597:GLU:HB3	2.15	0.47
1:D:528:THR:OG1	1:D:530:ARG:HD2	2.14	0.46
1:B:125:ASP:OD2	1:B:131:ARG:NH1	2.48	0.46
1:D:256:VAL:HA	1:D:260:TYR:HB2	1.96	0.46
1:B:112:ILE:HD13	1:B:118:LEU:HD23	1.98	0.46
1:D:531:THR:HG23	1:D:532:PHE:H	1.80	0.46
1:D:825:ASP:O	1:D:828:LYS:HB2	2.15	0.46
1:D:441:PRO:HB2	1:D:442:GLU:HB2	1.98	0.46
1:D:838:PRO:HG2	1:D:843:ILE:HD11	1.98	0.46
1:D:224:ASP:N	1:D:224:ASP:OD1	2.48	0.46
1:D:686:PHE:CZ	1:D:702:ILE:HG21	2.52	0.45
1:D:328:ASP:OD1	1:D:329:PHE:N	2.49	0.45
1:B:684:GLN:O	1:B:688:ARG:NH1	2.47	0.45
1:D:89:LEU:HD21	1:D:159:LEU:HD21	1.98	0.44
1:D:637:TYR:O	1:D:641:LEU:HB2	2.18	0.44
1:D:354:SER:HB3	1:D:357:SER:OG	2.17	0.44
1:B:342:LEU:O	1:B:638:TYR:OH	2.32	0.44
1:B:99:LYS:HD2	1:B:197:TYR:CZ	2.52	0.44
1:B:637:TYR:O	1:B:641:LEU:HB2	2.18	0.44
1:B:57:GLN:OE1	1:B:192:ASN:HB3	2.17	0.44
1:B:440:PHE:N	1:B:443:ASN:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:ALA:HB1	1:D:203:ILE:HD11	1.99	0.43
1:B:769:ILE:CG2	1:B:770:GLU:HA	2.46	0.43
1:B:99:LYS:HD2	1:B:197:TYR:CE2	2.52	0.43
1:B:704:THR:HG21	1:B:708:LEU:HD12	2.01	0.43
1:D:57:GLN:HB2	1:D:191:GLU:O	2.19	0.43
1:D:204:SER:HB2	1:D:209:THR:HG23	1.99	0.43
1:B:60:MET:HE2	1:B:194:LEU:HD13	2.01	0.43
1:D:394:SER:HA	1:D:425:LYS:NZ	2.33	0.43
1:D:839:ALA:O	1:D:843:ILE:HG12	2.19	0.43
1:B:763:PHE:HA	1:B:768:SER:CB	2.49	0.43
1:B:544:VAL:HA	1:B:674:ASP:O	2.19	0.42
1:D:60:MET:HE1	1:D:160:PRO:HD3	2.02	0.42
1:D:490:GLU:HG2	1:D:512:ARG:HH21	1.83	0.42
1:B:763:PHE:HA	1:B:768:SER:HB3	2.01	0.42
1:D:44:LEU:HD13	1:D:136:ILE:HG21	2.02	0.42
1:D:40:LEU:HD11	1:D:164:ILE:HG21	2.01	0.41
1:B:640:ASP:OD2	1:B:644:ARG:NE	2.50	0.41
1:B:847:ARG:NH2	1:B:886:GLN:OE1	2.40	0.41
1:D:65:ARG:HG3	1:D:81:TRP:CD2	2.54	0.41
1:D:476:LYS:NZ	1:D:478:ASP:OD2	2.48	0.41
1:B:679:TYR:CD1	1:B:718:LEU:HD12	2.56	0.40
1:B:60:MET:HE1	1:B:160:PRO:HD3	2.03	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	B	827/1038 (80%)	798 (96%)	26 (3%)	3 (0%)	39	68
1	D	825/1038 (80%)	785 (95%)	37 (4%)	3 (0%)	39	68
All	All	1652/2076 (80%)	1583 (96%)	63 (4%)	6 (0%)	39	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	810	SER
1	B	807	ILE
1	B	810	SER
1	D	807	ILE
1	B	769	ILE
1	D	769	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	B	690/927 (74%)	656 (95%)	34 (5%)	31	59
1	D	684/927 (74%)	647 (95%)	37 (5%)	27	54
All	All	1374/1854 (74%)	1303 (95%)	71 (5%)	29	56

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	21	ILE
1	B	40	LEU
1	B	65	ARG
1	B	71	LEU
1	B	89	LEU
1	B	118	LEU
1	B	165	GLU
1	B	169	ARG
1	B	221	ASN
1	B	240	LEU
1	B	253	LEU
1	B	282	ARG
1	B	298	LYS
1	B	301	SER
1	B	307	HIS
1	B	332	LYS

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Mol	Chain	Res	Type
1	B	336	VAL
1	B	346	THR
1	B	356	ASP
1	B	393	GLU
1	B	402	GLN
1	B	422	LEU
1	B	464	THR
1	B	641	LEU
1	B	652	LEU
1	B	655	VAL
1	B	688	ARG
1	B	718	LEU
1	B	722	LYS
1	B	731	LYS
1	B	765	ASP
1	B	781	LEU
1	B	840	ASP
1	D	21	ILE
1	D	26	THR
1	D	40	LEU
1	D	89	LEU
1	D	118	LEU
1	D	134	VAL
1	D	163	GLN
1	D	192	ASN
1	D	217	LYS
1	D	224	ASP
1	D	240	LEU
1	D	253	LEU
1	D	307	HIS
1	D	309	THR
1	D	336	VAL
1	D	356	ASP
1	D	393	GLU
1	D	402	GLN
1	D	422	LEU
1	D	425	LYS
1	D	443	ASN
1	D	464	THR
1	D	532	PHE
1	D	581	SER
1	D	626	ASN

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Mol	Chain	Res	Type
1	D	641	LEU
1	D	647	ASN
1	D	652	LEU
1	D	655	VAL
1	D	688	ARG
1	D	710	ARG
1	D	718	LEU
1	D	731	LYS
1	D	765	ASP
1	D	781	LEU
1	D	805	GLN
1	D	854	ARG

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

Mol	Chain	Res	Type
1	B	91	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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
2	ATP	B	1887	4	24,33,33	0.94	1 (4%)	31,52,52	1.91	5 (16%)
3	PO4	B	1888	-	4,4,4	0.45	0	6,6,6	0.27	0
3	PO4	B	1889	-	4,4,4	0.47	0	6,6,6	0.27	0
2	ATP	D	1887	4	24,33,33	0.94	1 (4%)	31,52,52	1.93	5 (16%)
3	PO4	D	1889	-	4,4,4	0.43	0	6,6,6	0.27	0
3	PO4	D	1890	-	4,4,4	0.48	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
2	ATP	B	1887	4	-	0/18/38/38	0/3/3/3
3	PO4	B	1888	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1889	-	-	0/0/0/0	0/0/0/0
2	ATP	D	1887	4	-	0/18/38/38	0/3/3/3
3	PO4	D	1889	-	-	0/0/0/0	0/0/0/0
3	PO4	D	1890	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1887	ATP	C5-C4	2.99	1.47	1.40
2	B	1887	ATP	C5-C4	2.99	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1887	ATP	N3-C2-N1	-6.84	123.66	128.89
2	B	1887	ATP	N3-C2-N1	-6.60	123.84	128.89
2	B	1887	ATP	PA-O3A-PB	-4.43	120.28	132.73
2	D	1887	ATP	PA-O3A-PB	-4.21	120.91	132.73
2	D	1887	ATP	C2'-C1'-N9	-3.39	109.12	114.29
2	B	1887	ATP	C2'-C1'-N9	-3.14	109.50	114.29
2	B	1887	ATP	C4-C5-N7	-2.99	106.73	109.48
2	D	1887	ATP	C4-C5-N7	-2.94	106.78	109.48
2	D	1887	ATP	PB-O3B-PG	-2.74	123.49	132.67
2	B	1887	ATP	PB-O3B-PG	-2.69	123.66	132.67

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
2	B	1887	ATP	1	0
2	D	1887	ATP	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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	837/1038 (80%)	0.83	100 (11%) 6 5	13, 33, 71, 121	0
1	D	835/1038 (80%)	0.98	137 (16%) 2 2	17, 40, 84, 114	0
All	All	1672/2076 (80%)	0.90	237 (14%) 4 3	13, 36, 78, 121	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	809	LEU	14.3
1	B	808	ASP	8.4
1	B	807	ILE	8.0
1	B	813	VAL	8.0
1	D	604	MET	7.8
1	D	534	GLY	7.5
1	D	566	ASN	7.4
1	D	809	LEU	7.4
1	D	768	SER	7.2
1	B	566	ASN	7.1
1	B	745	THR	6.9
1	B	814	ALA	6.9
1	B	812	PRO	6.7
1	D	533	PRO	6.6
1	D	818	PHE	6.5
1	D	816	GLU	6.5
1	D	808	ASP	6.2
1	D	565	ALA	6.1
1	B	564	ALA	6.1
1	B	568	SER	6.0
1	D	569	ALA	6.0
1	B	567	LYS	6.0
1	B	506	ALA	5.9
1	D	570	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	820	ALA	5.6
1	D	603	ALA	5.6
1	D	819	LYS	5.4
1	D	769	ILE	5.2
1	D	563	GLU	5.1
1	D	813	VAL	5.0
1	D	807	ILE	5.0
1	B	498	LEU	5.0
1	D	767	THR	4.9
1	B	170	GLY	4.9
1	B	826	ASP	4.9
1	D	773	LYS	4.8
1	D	811	ASP	4.7
1	D	506	ALA	4.7
1	D	495	GLU	4.6
1	B	855	ASP	4.6
1	D	853	ILE	4.6
1	D	511	MET	4.6
1	D	814	ALA	4.6
1	B	604	MET	4.4
1	D	441	PRO	4.4
1	D	623	PHE	4.4
1	D	772	GLU	4.4
1	B	565	ALA	4.3
1	D	815	VAL	4.3
1	D	562	GLU	4.3
1	B	722	LYS	4.3
1	D	810	SER	4.3
1	D	855	ASP	4.3
1	B	511	MET	4.2
1	B	723	ASN	4.2
1	D	717	THR	4.1
1	B	744	ALA	4.1
1	D	723	ASN	4.1
1	D	567	LYS	4.1
1	B	818	PHE	4.0
1	D	535	SER	4.0
1	D	714	ASP	4.0
1	B	606	SER	3.9
1	D	502	GLU	3.9
1	D	421	ASN	3.9
1	B	718	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	774	GLU	3.9
1	B	621	SER	3.9
1	D	743	ALA	3.8
1	B	494	ASP	3.8
1	D	499	SER	3.8
1	B	356	ASP	3.8
1	D	568	SER	3.8
1	D	582	PHE	3.8
1	D	571	TYR	3.8
1	B	571	TYR	3.7
1	D	564	ALA	3.7
1	D	479	TYR	3.6
1	D	355	PRO	3.6
1	D	602	SER	3.6
1	B	563	GLU	3.6
1	D	560	LEU	3.6
1	B	819	LYS	3.5
1	B	827	GLU	3.5
1	D	498	LEU	3.5
1	D	744	ALA	3.5
1	B	508	LEU	3.4
1	B	502	GLU	3.4
1	B	825	ASP	3.4
1	B	570	THR	3.4
1	D	765	ASP	3.4
1	D	406	ILE	3.4
1	D	820	ALA	3.4
1	B	496	LYS	3.3
1	B	824	VAL	3.3
1	D	817	LYS	3.3
1	D	764	PRO	3.3
1	D	365	ALA	3.3
1	D	745	THR	3.3
1	B	509	HIS	3.3
1	D	374	ASP	3.3
1	B	618	GLU	3.2
1	B	854	ARG	3.2
1	B	290	SER	3.2
1	D	601	THR	3.2
1	D	622	HIS	3.2
1	D	387	ASN	3.2
1	B	743	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	445	LEU	3.1
1	D	572	LYS	3.1
1	B	446	GLY	3.1
1	D	170	GLY	3.1
1	B	449	THR	3.1
1	B	742	ASP	3.1
1	D	806	GLN	3.1
1	D	679	TYR	3.1
1	D	505	GLN	3.1
1	D	605	ASP	3.1
1	B	806	GLN	3.1
1	D	500	ALA	3.1
1	D	812	PRO	3.1
1	B	770	GLU	3.1
1	B	444	ALA	3.0
1	B	605	ASP	3.0
1	D	822	HIS	3.0
1	D	824	VAL	3.0
1	B	150	TYR	3.0
1	D	344	TYR	3.0
1	B	357	SER	3.0
1	D	440	PHE	3.0
1	B	441	PRO	3.0
1	D	766	PRO	3.0
1	D	501	ALA	2.9
1	D	295	ASN	2.9
1	D	850	TYR	2.9
1	D	606	SER	2.9
1	B	623	PHE	2.9
1	B	829	PHE	2.9
1	D	721	ASP	2.8
1	D	32	SER	2.8
1	D	852	ASP	2.8
1	B	190	SER	2.8
1	D	763	PHE	2.8
1	D	508	LEU	2.8
1	D	375	ASP	2.8
1	B	355	PRO	2.7
1	B	535	SER	2.7
1	B	627	PHE	2.7
1	D	770	GLU	2.7
1	B	291	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	533	PRO	2.7
1	B	505	GLN	2.6
1	D	444	ALA	2.6
1	B	817	LYS	2.6
1	B	447	SER	2.6
1	D	28	ASP	2.6
1	B	534	GLY	2.6
1	D	496	LYS	2.6
1	B	874	ASP	2.5
1	D	493	THR	2.5
1	D	608	ALA	2.5
1	B	501	ALA	2.5
1	B	811	ASP	2.5
1	D	515	GLU	2.5
1	D	356	ASP	2.5
1	D	821	GLU	2.5
1	D	416	GLY	2.5
1	B	620	ASN	2.5
1	B	626	ASN	2.5
1	D	189	ASN	2.5
1	D	747	GLU	2.5
1	B	375	ASP	2.5
1	B	852	ASP	2.5
1	B	541	MET	2.4
1	D	410	CYS	2.4
1	B	560	LEU	2.4
1	D	364	THR	2.4
1	D	447	SER	2.4
1	D	388	ASN	2.4
1	D	650	ILE	2.4
1	D	110	ASP	2.4
1	D	618	GLU	2.3
1	B	189	ASN	2.3
1	B	420	LYS	2.3
1	D	531	THR	2.3
1	D	536	LYS	2.3
1	B	218	ARG	2.3
1	B	721	ASP	2.3
1	D	760	GLU	2.3
1	D	856	TRP	2.3
1	D	838	PRO	2.3
1	B	219	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	292	THR	2.3
1	B	661	THR	2.3
1	D	851	ASN	2.3
1	D	21	ILE	2.3
1	D	489	LEU	2.2
1	D	293	ALA	2.2
1	B	572	LYS	2.2
1	D	414	GLN	2.2
1	D	561	GLN	2.2
1	D	598	THR	2.2
1	B	717	THR	2.2
1	D	321	ALA	2.2
1	D	494	ASP	2.2
1	D	825	ASP	2.2
1	B	856	TRP	2.2
1	D	832	LEU	2.2
1	B	495	GLU	2.2
1	B	816	GLU	2.2
1	D	614	ALA	2.2
1	D	449	THR	2.2
1	B	581	SER	2.2
1	D	452	SER	2.2
1	D	649	ASP	2.2
1	B	289	SER	2.1
1	B	769	ILE	2.1
1	B	751	GLY	2.1
1	D	285	TRP	2.1
1	D	445	LEU	2.1
1	D	559	ARG	2.1
1	B	660	LEU	2.1
1	B	815	VAL	2.1
1	D	581	SER	2.1
1	B	828	LYS	2.1
1	B	851	ASN	2.1
1	D	859	ARG	2.1
1	B	830	ALA	2.1
1	D	621	SER	2.1
1	D	541	MET	2.1
1	D	442	GLU	2.1
1	D	624	LYS	2.0
1	B	320	ALA	2.0
1	D	422	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	607	SER	2.0
1	B	257	LEU	2.0
1	B	448	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	D	1889	5/5	0.86	0.17	-0.41	36,53,55,82	0
3	PO4	B	1889	5/5	0.90	0.16	-0.61	52,55,69,83	0
3	PO4	D	1890	5/5	0.98	0.14	-1.03	16,17,21,23	0
2	ATP	D	1887	31/31	0.97	0.17	-1.09	13,21,27,33	0
2	ATP	B	1887	31/31	0.97	0.16	-1.33	11,18,23,25	0
3	PO4	B	1888	5/5	0.98	0.13	-1.37	24,24,27,32	0
4	MG	B	1890	1/1	0.92	0.34	-	23,23,23,23	0
4	MG	D	1886	1/1	0.87	0.27	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.