



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 12:27 am BST

PDB ID : 1FRV
Title : CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDROGENASE
Authors : Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C.
Deposited on : 1996-03-28
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

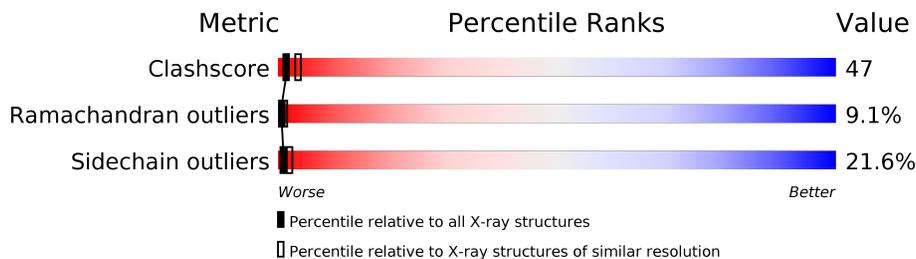
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	37% 44% 17% ..
1	C	264	29% 52% 16% ..
2	B	536	32% 47% 18% ..
2	D	536	18% 56% 22% ..

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
3	SF4	C	265	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12268 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.

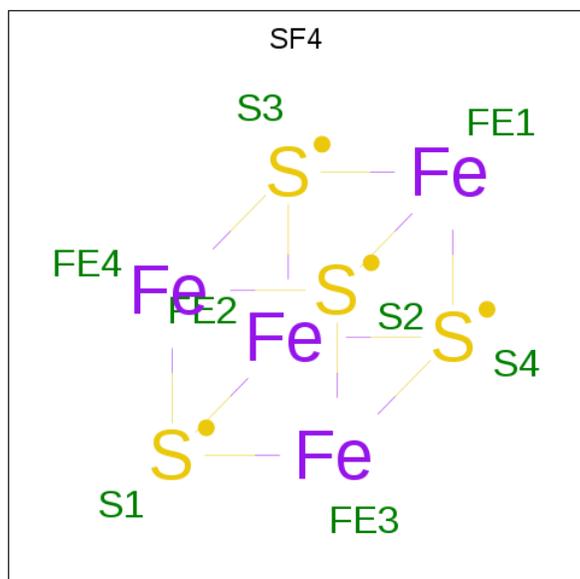
- Molecule 1 is a protein called HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	Total 1961	C 1247	N 328	O 367	S 19	0	0	0
1	C	262	Total 1961	C 1247	N 328	O 367	S 19	0	0	0

- Molecule 2 is a protein called HYDROGENASE.

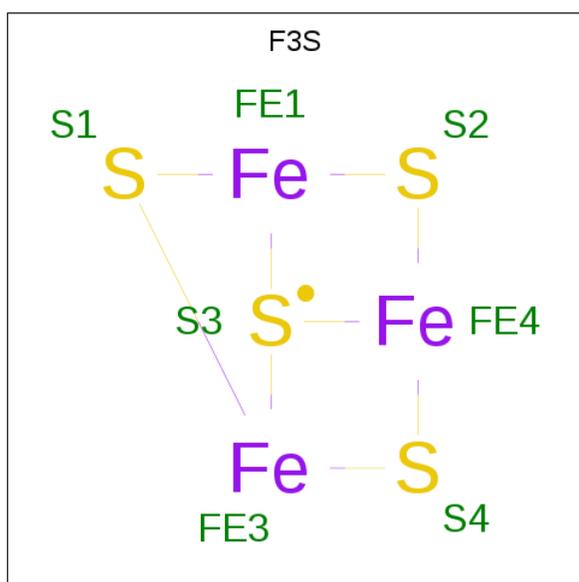
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	530	Total 4145	C 2645	N 725	O 758	S 17	0	0	0
2	D	530	Total 4145	C 2645	N 725	O 758	S 17	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).

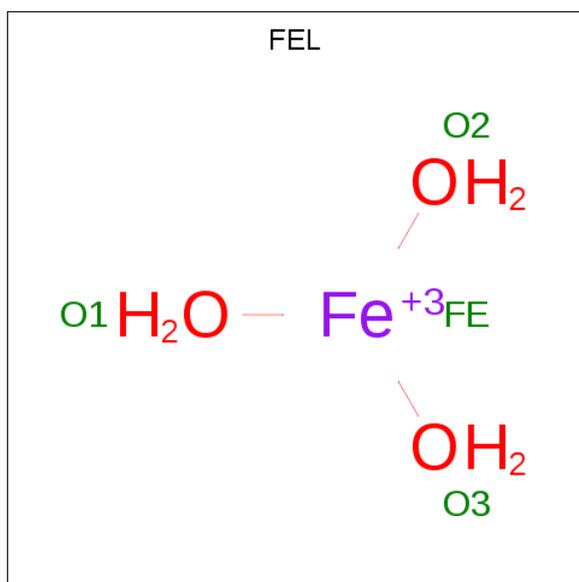


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		

- Molecule 6 is HYDRATED FE (three-letter code: FEL) (formula: FeH₆O₃).



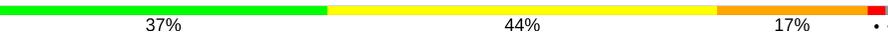
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	O	0	0
			4	1	3		
6	D	1	Total	Fe	O	0	0
			4	1	3		

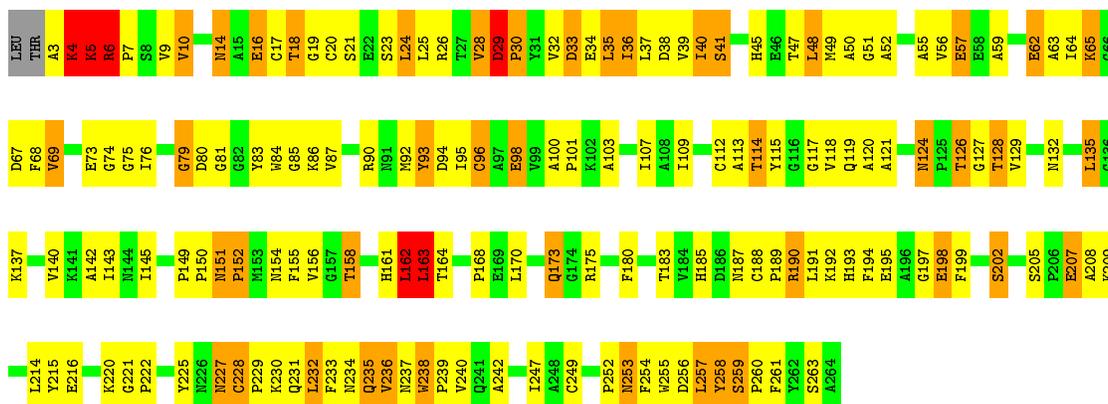
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

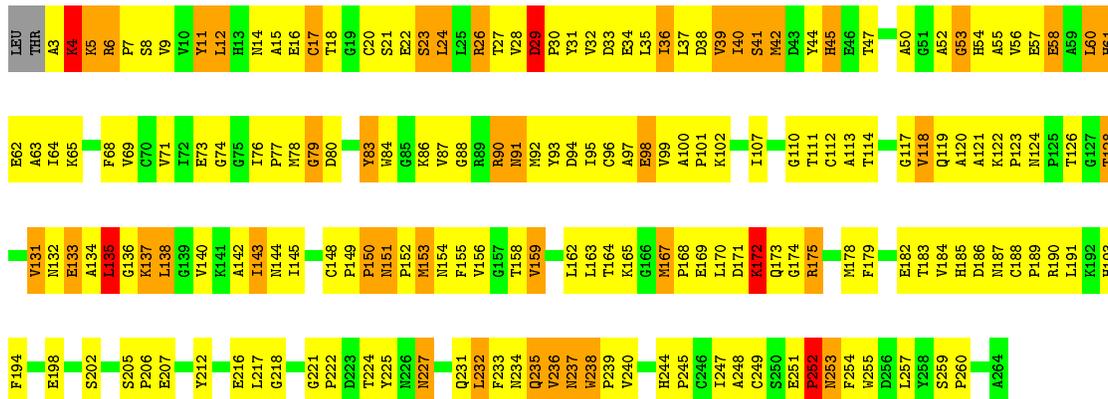
- Molecule 1: HYDROGENASE

Chain A: 



- Molecule 1: HYDROGENASE

Chain C: 



- Molecule 2: HYDROGENASE

Chain B: 

MET	K8	V71	V70	T69	V67	C66	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644	K645	K646	K647	K648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713	K714	K715	K716	K717	K718	K719	K720	K721	K722	K723	K724	K725	K726	K727	K728	K729	K730	K731	K732	K733	K734	K735	K736	K737	K738	K739	K740	K741	K742	K743	K744	K745	K746	K747	K748	K749	K750	K751	K752	K753	K754	K755	K756	K757	K758	K759	K760	K761	K762	K763	K764	K765	K766	K767	K768	K769	K770	K771	K772	K773	K774	K775	K776	K777	K778	K779	K780	K781	K782	K783	K784	K785	K786	K787	K788	K789	K790	K791	K792	K793	K794	K795	K796	K797	K798	K799	K800	K801	K802	K803	K804	K805	K806	K807	K808	K809	K810	K811	K812	K813	K814	K815	K816	K817	K818	K819	K820	K821	K822	K823	K824	K825	K826	K827	K828	K829	K830	K831	K832	K833	K834	K835	K836	K837	K838	K839	K840	K841	K842	K843	K844	K845	K846	K847	K848	K849	K850	K851	K852	K853	K854	K855	K856	K857	K858	K859	K860	K861	K862	K863	K864	K865	K866	K867	K868	K869	K870	K871	K872	K873	K874	K875	K876	K877	K878	K879	K880	K881	K882	K883	K884	K885	K886	K887	K888	K889	K890	K891	K892	K893	K894	K895	K896	K897	K898	K899	K900	K901	K902	K903	K904	K905	K906	K907	K908	K909	K910	K911	K912	K913	K914	K915	K916	K917	K918	K919	K920	K921	K922	K923	K924	K925	K926	K927	K928	K929	K930	K931	K932	K933	K934	K935	K936	K937	K938	K939	K940	K941	K942	K943	K944	K945	K946	K947	K948	K949	K950	K951	K952	K953	K954	K955	K956	K957	K958	K959	K960	K961	K962	K963	K964	K965	K966	K967	K968	K969	K970	K971	K972	K973	K974	K975	K976	K977	K978	K979	K980	K981	K982	K983	K984	K985	K986	K987	K988	K989	K990	K991	K992	K993	K994	K995	K996	K997	K998	K999	Q103	Y104	M105	H106	D107	H108	L109	V110	H111	F112	Y113	H114	L115	K50	G51	R52	D53	P54	L55	L56	L57	L58	L59	L60	L61	L62	L63	L64	L65	L66	L67	L68	L69	L70	L71	L72	L73	L74	L75	L76	L77	L78	L79	L80	L81	L82	L83	L84	L85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	M100	R101	G102	H103	D104	H105	L106	L107	L108	L109	L110	L111	L112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	M200	R201	G202	H203	D204	H205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L38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L443	L444	Y444	T445	D446	W447	Q448	Y449	F450	T451	E452	S453	Q454	G455	V456	G457	F458	W459	W460	M461	F462	R463	G464	M465	L466	S467	E468	W469	I470	V471	Q472	R473	G474	G475	K476	I477	E478	W479	F480	Q481	H482	W483	W484	P485	S486	E487	W488	M489	L490	G491	E492	R493	C494	A495	E496	R497	E498	L499	S500	A501	V502
E503	I506	I507	G508	T509	P510	I511	A512	D513	P514	K515	R516	P517	V518	E519	I520	L521	R522	T523	V524	H525	S526	Y527	D528	E529	C530	I531	A532	C533	G534	Y535	H536																													

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 93.90Å 69.20Å 89.80° 102.90° 90.80°	Depositor
Resolution (Å)	8.00 – 2.85	Depositor
% Data completeness (in resolution range)	85.3 (8.00-2.85)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12268	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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: NI, SF4, F3S, FEL

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	0.84	0/2014	1.43	12/2738 (0.4%)
1	C	0.84	0/2014	1.44	11/2738 (0.4%)
2	B	0.81	0/4251	1.45	37/5782 (0.6%)
2	D	0.81	0/4251	1.45	36/5782 (0.6%)
All	All	0.82	0/12530	1.45	96/17040 (0.6%)

There are no bond length outliers.

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	C	190	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	B	414	ARG	NE-CZ-NH1	11.16	125.88	120.30
2	D	16	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	74	GLY	N-CA-C	10.34	138.94	113.10

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	1961	0	1879	155	0
1	C	1961	0	1879	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4145	0	4073	362	1
2	D	4145	0	4073	487	1
3	A	16	0	0	2	0
3	C	16	0	0	3	0
4	A	7	0	0	0	0
4	C	7	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
All	All	12268	0	11904	1142	1

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 47.

The worst 5 of 1142 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)
2:B:308:LEU:HD21	2:B:405:PHE:HZ	1.15	1.07
2:D:14:ILE:HG13	2:D:21:LEU:HD13	1.30	1.07
1:C:29:ASP:HB3	1:C:30:PRO:HD3	1.30	1.06
2:D:27:VAL:HG22	2:D:32:ILE:HA	1.38	1.02
1:A:29:ASP:HB3	1:A:30:PRO:HD3	1.41	1.01

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:ASP:OD2	2:D:31:LYS:NZ[1_565]	2.18	0.02

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	A	260/264 (98%)	198 (76%)	42 (16%)	20 (8%)	1	2
1	C	260/264 (98%)	192 (74%)	43 (16%)	25 (10%)	0	1
2	B	528/536 (98%)	387 (73%)	94 (18%)	47 (9%)	1	1
2	D	528/536 (98%)	379 (72%)	97 (18%)	52 (10%)	0	1
All	All	1576/1600 (98%)	1156 (73%)	276 (18%)	144 (9%)	1	1

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	29	ASP
1	A	41	SER
1	A	79	GLY
2	B	35	ALA

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	A	205/211 (97%)	160 (78%)	45 (22%)	1	2
1	C	205/211 (97%)	161 (78%)	44 (22%)	1	2
2	B	431/441 (98%)	346 (80%)	85 (20%)	1	3
2	D	431/441 (98%)	330 (77%)	101 (23%)	1	1
All	All	1272/1304 (98%)	997 (78%)	275 (22%)	1	2

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	496	GLU
1	C	128	THR
2	D	446	ASP
2	B	518	VAL
1	C	32	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	460	ASN
2	B	504	GLN
2	D	479	ASN
2	B	479	ASN
1	C	13	HIS

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	SF4	A	265	1	0,12,12	0.00	-	-	-	
3	SF4	C	265	1	0,12,12	0.00	-	-	-	
4	F3S	A	266	1	0,9,9	0.00	-	-	-	
4	F3S	C	266	1	0,9,9	0.00	-	-	-	
6	FEL	D	537	2	0,3,3	0.00	-	-	-	
3	SF4	C	267	1	0,12,12	0.00	-	-	-	
6	FEL	B	537	2	0,3,3	0.00	-	-	-	
3	SF4	A	267	1	0,12,12	0.00	-	-	-	

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	SF4	A	265	1	-	-	0/6/5/5
3	SF4	C	265	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
4	F3S	C	266	1	-	-	0/3/3/3
3	SF4	C	267	1	-	-	0/6/5/5
3	SF4	A	267	1	-	-	0/6/5/5

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	265	SF4	1	0
3	C	265	SF4	2	0
3	C	267	SF4	1	0
3	A	267	SF4	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.