



wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 11:54 AM GMT

PDB ID : 2D5H
Title : Crystal Structure of Recombinant Soybean Proglycinin A3B4 subunit, its Comparison with Mature Glycinin A3B4 subunit, Responsible for Hexamer Assembly
Authors : Itoh, T.; Adachi, M.; Masuda, T.; Mikami, B.; Utsumi, S.
Deposited on : 2005-11-01
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

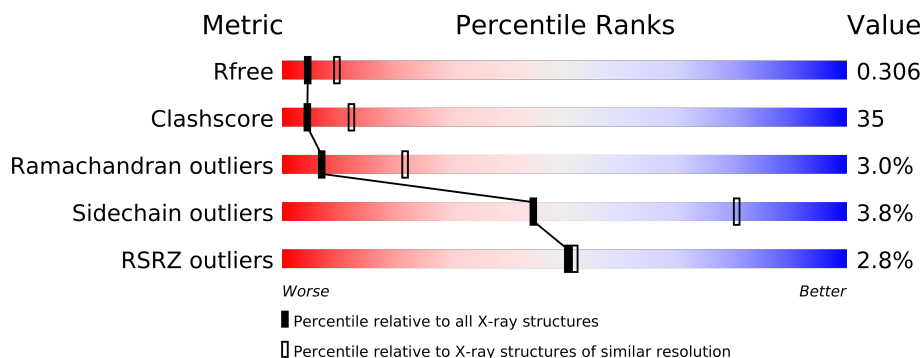
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	493	
1	B	493	
1	C	493	
1	D	493	
1	E	493	
1	F	493	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CO3	A	501	-	X
2	CO3	B	502	-	X

2 Entry composition

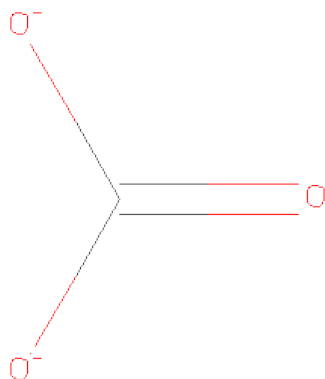
There are 3 unique types of molecules in this entry. The entry contains 17703 atoms, of which 0 are hydrogen and 0 are deuterium.

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 glycinin A3B4 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2937	1844	523	562	8			
1	B	372	Total	C	N	O	S	0	0	0
			2920	1835	520	557	8			
1	C	370	Total	C	N	O	S	0	0	0
			2905	1827	517	553	8			
1	D	377	Total	C	N	O	S	0	0	0
			2967	1861	529	569	8			
1	E	380	Total	C	N	O	S	0	0	0
			2981	1872	530	571	8			
1	F	377	Total	C	N	O	S	0	0	0
			2963	1860	528	567	8			

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 1 3	0	0
2	B	1	Total C O 4 1 3	0	0
2	C	1	Total C O 4 1 3	0	0
2	D	1	Total C O 4 1 3	0	0
2	E	1	Total C O 4 1 3	0	0
2	F	1	Total C O 4 1 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

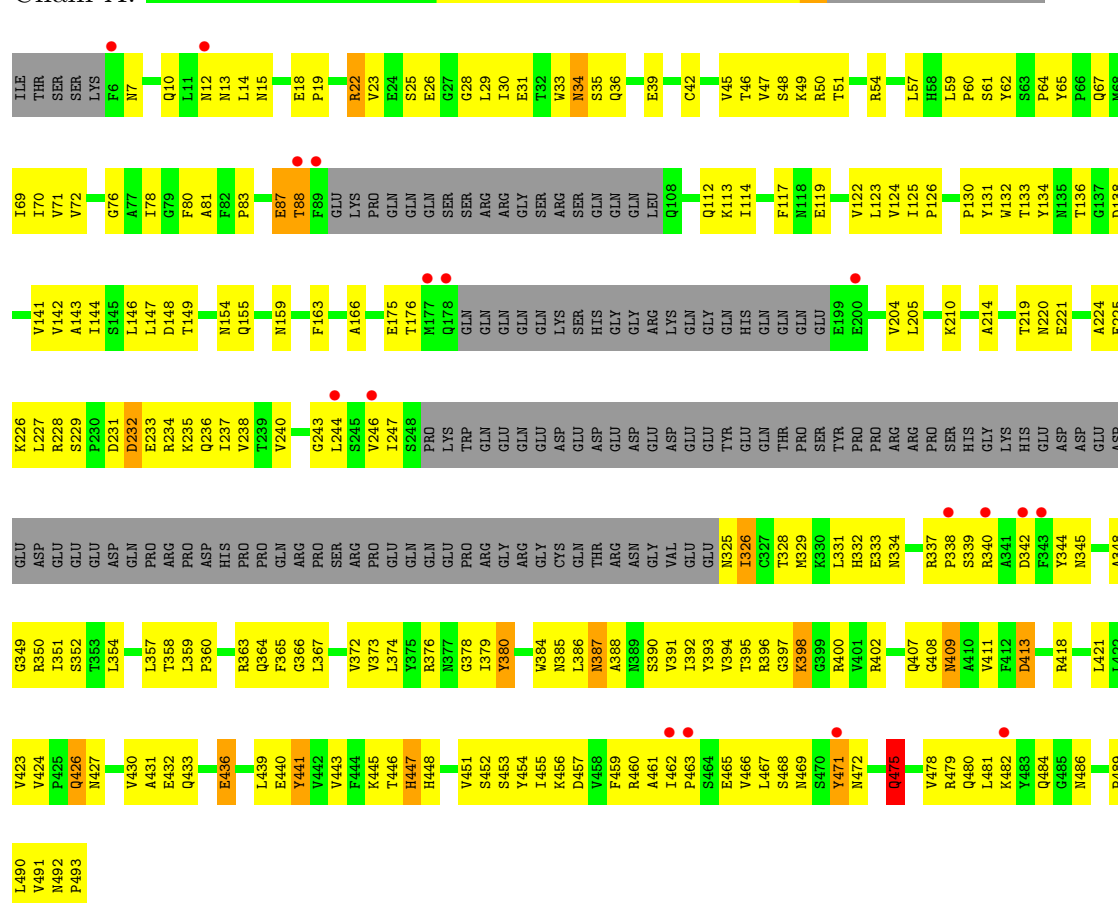
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

3 Residue-property plots

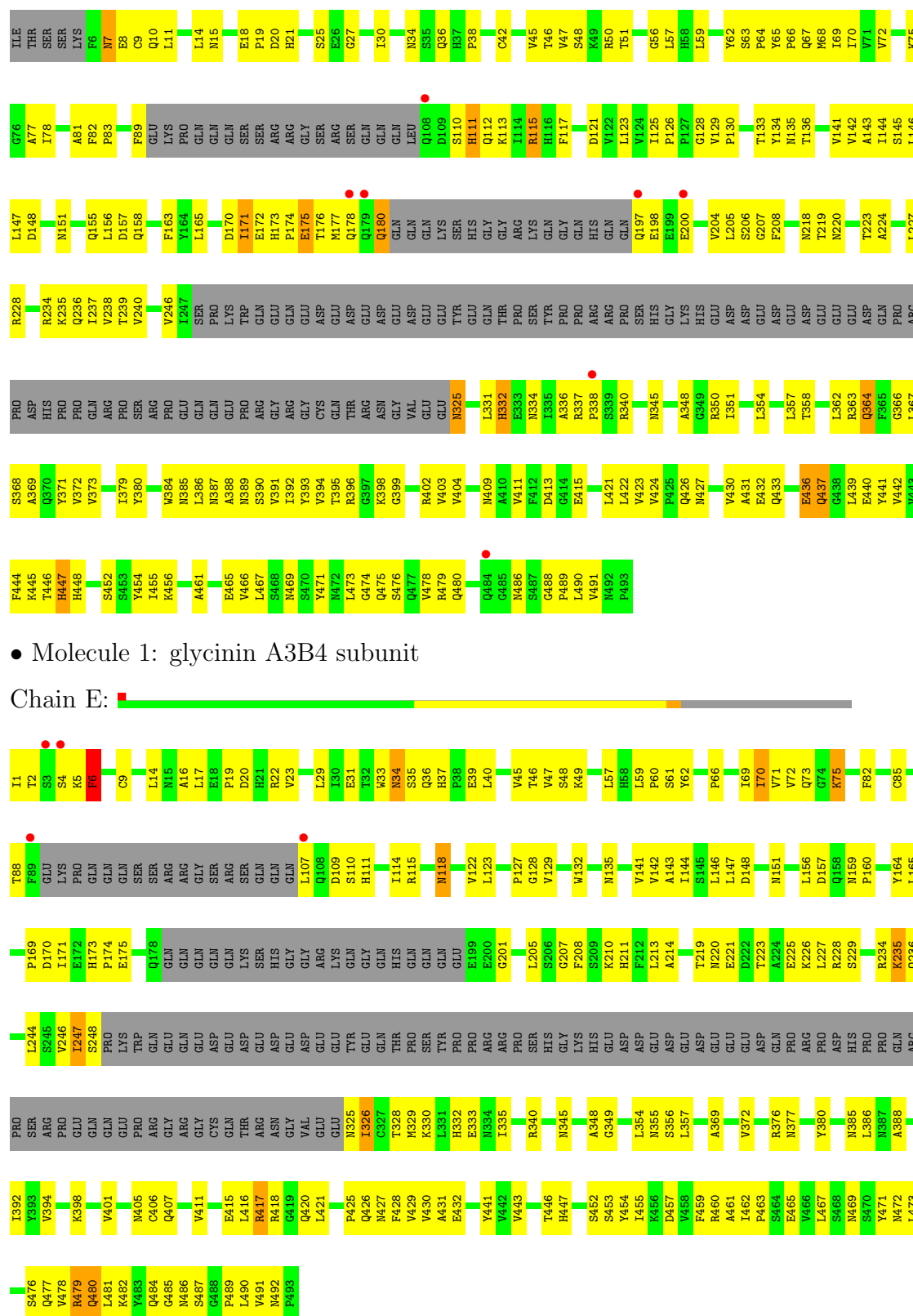
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: glycinin A3B4 subunit

Chain A:







A431	A432	Q433	G434	G435	E436	L439	E440	Y441	K445	Y454	I455	K456	D457	V458	A461	I462	P463	S464	E465	V466	L467	S468	Y471	N472	L473	Q474	Q477	V478	R479	Q480	L481	K482	Y483	N486	L490	V491	P493														
G349	R350	I351	N355	S356	L357	L362	L367	V373	Y380	N385	L386	N387	A388	N389	S390	V391	I392	Y393	V394	T395	R396	G397	K398	G399	R400	V401	R402	V403	V404	N405	C406	Q407	G408	N409	A410	V411	F412	D413	L416	R417	R418	L421	L422	V423	V424	P425	Q426	N427	F428	V429	V430
ASP	GLU	GLU	ASP	GLU	GLU	ASP	GLN	PRO	ARG	PRO	GLN	ARG	PRO	SER	ARG	PRO	GLN	ARG	PRO	PRO	ARG	GLU	GLN	GLU	GLU	CYS	GLN	THR	ASN	VAL	GLY	GLU	GLU	N325	T328	M329	K330	L331	H332	E333	N334	I335	A336	R337	R340	F343	Y344	N345	A348		
D222	T223	A224	E225	K226	P230	D231	E233	K234	Q236	T237	V238	V240	G243	L244	S245	V246	I247	S248	PRO	LYS	THR	GLN	LYS	THR	GLY	GLN	GLY	ASP	GLU	GLU	GLU	GLU	TYR	GLN	GLN	THR	PRO	SER	TYR	PRO	ARG	ARG	PRO	PRO	HIS	GLY	LYS	HIS	GLU	ASP	
D148	T149	S150	N151	F152	M153	N154	Q155	P159	P160	F163	Y164	G167	D170	I171	T176	Q179	GLN	GLN	GLN	GLN	LYS	S110	SER	H111	Q112	K113	I114	R115	F116	F117	N118	D121	V122	L123	V124	I125	P126	P127	G128	V129	P130	V131	V132	T133	Y134	N135	T136	V141	I144	S145	L147
ILE	THR	SER	SER	LYS	F6	N7	L14	P19	D20	H21	S25	E26	G27	G28	L29	I30	E31	N34	S35	G36	H37	P38	L40	Q41	Q42	V45	T46	K49	R50	T51	L52	N53	L59	P60	Y62	Y65	P66	Q67	M68	I69	I70	V71	V72	G76	A77	I78	A81				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.38Å 223.74Å 88.66Å 90.00° 119.85° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 45.36 – 2.78	Depositor EDS
% Data completeness (in resolution range)	85.1 (15.00-2.80) 83.1 (45.36-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.325 0.231 , 0.306	Depositor DCC
R_{free} test set	5961 reflections (10.13%)	DCC
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 7.6	EDS
Estimated twinning fraction	0.047 for -h-l,k,h 0.047 for l,k,-h-l 0.034 for -h-l,-k,l 0.035 for l,-k,h 0.034 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63184 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17703	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, CO3, MG

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	0.27	0/2995	0.49	0/4068
1	B	0.27	0/2978	0.49	0/4045
1	C	0.27	0/2963	0.50	0/4025
1	D	0.26	0/3025	0.51	0/4108
1	E	0.28	0/3039	0.52	0/4127
1	F	0.27	0/3021	0.51	0/4103
All	All	0.27	0/18021	0.50	0/24476

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2937	0	2841	248	0
1	B	2920	0	2830	251	0
1	C	2905	0	2817	265	0
1	D	2967	0	2867	193	0
1	E	2981	0	2897	183	0
1	F	2963	0	2868	211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	B	4	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	17703	0	17120	1233	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

The worst 5 of 1233 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:334:ASN:HD22	1:C:337:ARG:HG2	1.17	1.08
1:F:159:ASN:HD22	1:F:176:THR:HG22	1.20	1.06
1:F:115:ARG:HH22	1:F:331:LEU:HD12	1.20	1.04
1:E:247:ILE:HG12	1:E:248:SER:H	1.19	1.04
1:B:159:ASN:HD22	1:B:176:THR:HG22	1.29	0.98

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	365/493 (74%)	302 (83%)	54 (15%)	9 (2%)	9	28
1	B	363/493 (74%)	297 (82%)	54 (15%)	12 (3%)	6	19
1	C	361/493 (73%)	291 (81%)	51 (14%)	19 (5%)	3	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	368/493 (75%)	307 (83%)	54 (15%)	7 (2%)	12	37
1	E	371/493 (75%)	311 (84%)	54 (15%)	6 (2%)	14	44
1	F	368/493 (75%)	311 (84%)	44 (12%)	13 (4%)	6	18
All	All	2196/2958 (74%)	1819 (83%)	311 (14%)	66 (3%)	7	22

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	GLN
1	B	426	GLN
1	C	245	SER
1	C	418	ARG
1	D	171	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/435 (74%)	310 (96%)	14 (4%)	40	76
1	B	322/435 (74%)	313 (97%)	9 (3%)	56	88
1	C	320/435 (74%)	305 (95%)	15 (5%)	36	73
1	D	327/435 (75%)	314 (96%)	13 (4%)	42	79
1	E	330/435 (76%)	318 (96%)	12 (4%)	47	82
1	F	327/435 (75%)	316 (97%)	11 (3%)	49	84
All	All	1950/2610 (75%)	1876 (96%)	74 (4%)	44	80

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	371	TYR
1	D	121	ASP
1	F	200	GLU
1	C	380	TYR
1	C	436	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	178	GLN
1	D	12	ASN
1	F	334	ASN
1	C	332	HIS
1	C	409	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 non-standard protein/DNA/RNA residues 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
1	CSD	A	406	1	7,7,8	6.80	2 (28%)	6,8,10	1.79	2 (33%)
1	CSD	B	406	1	7,7,8	6.82	2 (28%)	6,8,10	1.95	3 (50%)
1	CSD	C	406	1	7,7,8	6.69	2 (28%)	6,8,10	1.68	3 (50%)
1	CSD	D	406	1	7,7,8	6.71	2 (28%)	6,8,10	1.82	3 (50%)
1	CSD	E	406	1	7,7,8	6.64	2 (28%)	6,8,10	1.88	2 (33%)
1	CSD	F	406	1	7,7,8	6.76	2 (28%)	6,8,10	2.19	3 (50%)

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
1	CSD	A	406	1	-	0/3/6/8	0/0/0/0
1	CSD	B	406	1	-	0/3/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	C	406	1	-	0/3/6/8	0/0/0/0
1	CSD	D	406	1	-	0/3/6/8	0/0/0/0
1	CSD	E	406	1	-	0/3/6/8	0/0/0/0
1	CSD	F	406	1	-	0/3/6/8	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	406	CSD	O-C	17.81	1.23	1.11
1	A	406	CSD	O-C	17.76	1.23	1.11
1	F	406	CSD	O-C	17.68	1.23	1.11
1	D	406	CSD	O-C	17.54	1.23	1.11
1	C	406	CSD	O-C	17.53	1.23	1.11

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	406	CSD	CA-CB-SG	3.78	116.21	110.82
1	B	406	CSD	CA-CB-SG	3.43	115.71	110.82
1	E	406	CSD	CA-CB-SG	3.24	115.44	110.82
1	A	406	CSD	CA-CB-SG	3.08	115.21	110.82
1	D	406	CSD	CA-CB-SG	2.64	114.58	110.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 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	CO3	A	501	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	B	502	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	C	503	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	D	504	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	E	505	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	F	506	-	0,3,3	0.00	-	0,3,3	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
2	CO3	A	501	-	-	0/0/0/0	0/0/0/0
2	CO3	B	502	-	-	0/0/0/0	0/0/0/0
2	CO3	C	503	-	-	0/0/0/0	0/0/0/0
2	CO3	D	504	-	-	0/0/0/0	0/0/0/0
2	CO3	E	505	-	-	0/0/0/0	0/0/0/0
2	CO3	F	506	-	-	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.

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 ⓘ

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	A	374/493 (75%)	0.09	17 (4%) 32 33	13, 37, 54, 62	0
1	B	372/493 (75%)	0.02	11 (2%) 48 49	6, 37, 56, 63	0
1	C	370/493 (75%)	0.28	21 (5%) 23 23	7, 39, 54, 66	0
1	D	377/493 (76%)	-0.37	7 (1%) 64 64	6, 18, 46, 57	0
1	E	380/493 (77%)	-0.42	4 (1%) 77 78	6, 13, 43, 58	0
1	F	377/493 (76%)	-0.38	3 (0%) 83 83	6, 18, 45, 57	0
All	All	2250/2958 (76%)	-0.13	63 (2%) 50 52	6, 28, 52, 66	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	THR	7.8
1	C	246	VAL	5.2
1	C	89	PHE	4.9
1	B	437	GLN	4.1
1	E	89	PHE	3.8

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	F	406	8/9	0.17	0.17	5,8,30,57	0
1	CSD	A	406	8/9	0.16	0.07	30,41,46,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CSD	E	406	8/9	0.14	-0.17	5,7,45,53	0
1	CSD	C	406	8/9	0.16	-0.34	31,38,58,62	0
1	CSD	B	406	8/9	0.13	-1.06	39,44,63,73	0
1	CSD	D	406	8/9	0.09	-3.08	5,13,23,38	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CO3	B	502	4/4	0.26	5.98	12,22,39,45	0
2	CO3	A	501	4/4	0.28	2.01	14,35,39,41	0
2	CO3	C	503	4/4	0.25	1.79	36,40,41,42	0
2	CO3	F	506	4/4	0.20	1.27	5,5,18,21	0
2	CO3	E	505	4/4	0.17	1.19	5,5,10,17	0
3	MG	E	605	1/1	0.14	-0.18	5,5,5,5	0
3	MG	B	602	1/1	0.21	-0.61	41,41,41,41	0
2	CO3	D	504	4/4	0.13	-0.88	5,19,20,21	0
3	MG	D	604	1/1	0.13	-1.17	17,17,17,17	0
3	MG	F	606	1/1	0.13	-1.23	8,8,8,8	0
3	MG	C	603	1/1	0.16	-1.55	21,21,21,21	0
3	MG	A	601	1/1	0.11	-2.42	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.