wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 12:44 AM EDT

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 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

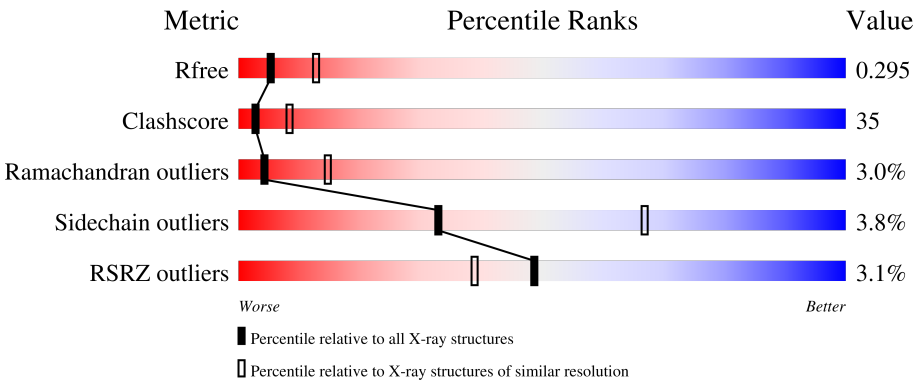
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of 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 <=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	A	493	4% 32% 40% • 24%
1	B	493	2% 33% 39% • 25%
1	C	493	5% 26% 44% 5% 25%
1	D	493	% 36% 38% • 24%
1	E	493	% 40% 34% • 23%

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Mol	Chain	Length	Quality of chain
1	F	493	% 36% 36% • 24%

2 Entry composition (i)

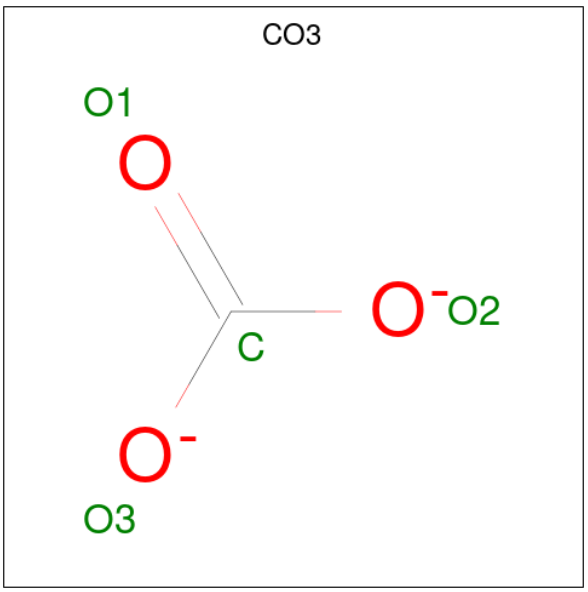
There are 3 unique types of molecules in this entry. The entry contains 17703 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycinin A3B4 subunit.

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

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

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

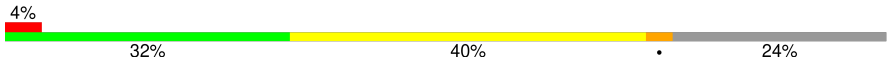
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0

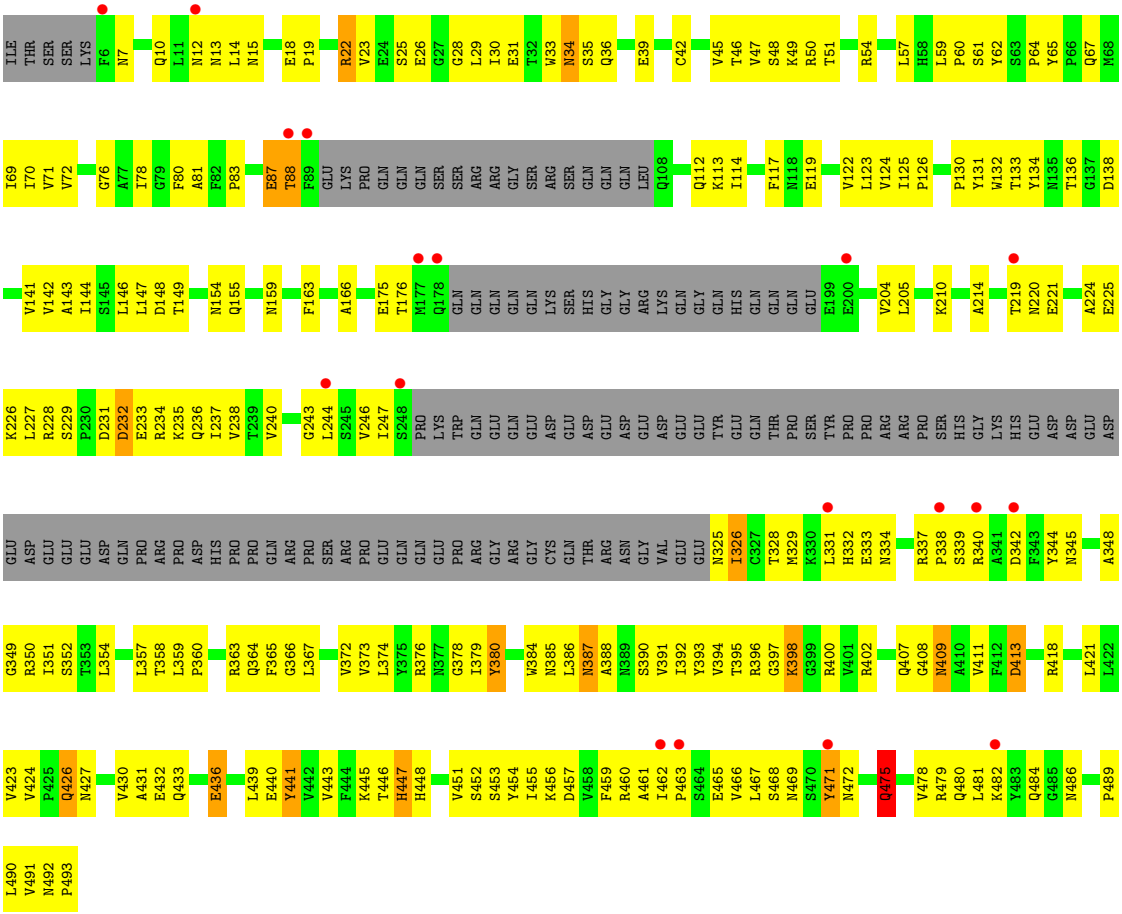
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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

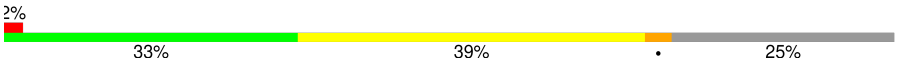
Chain A:

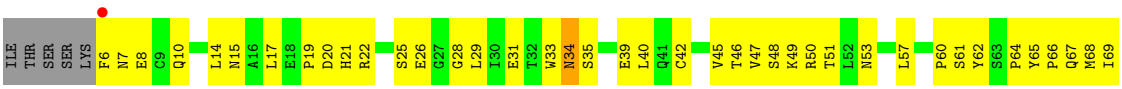


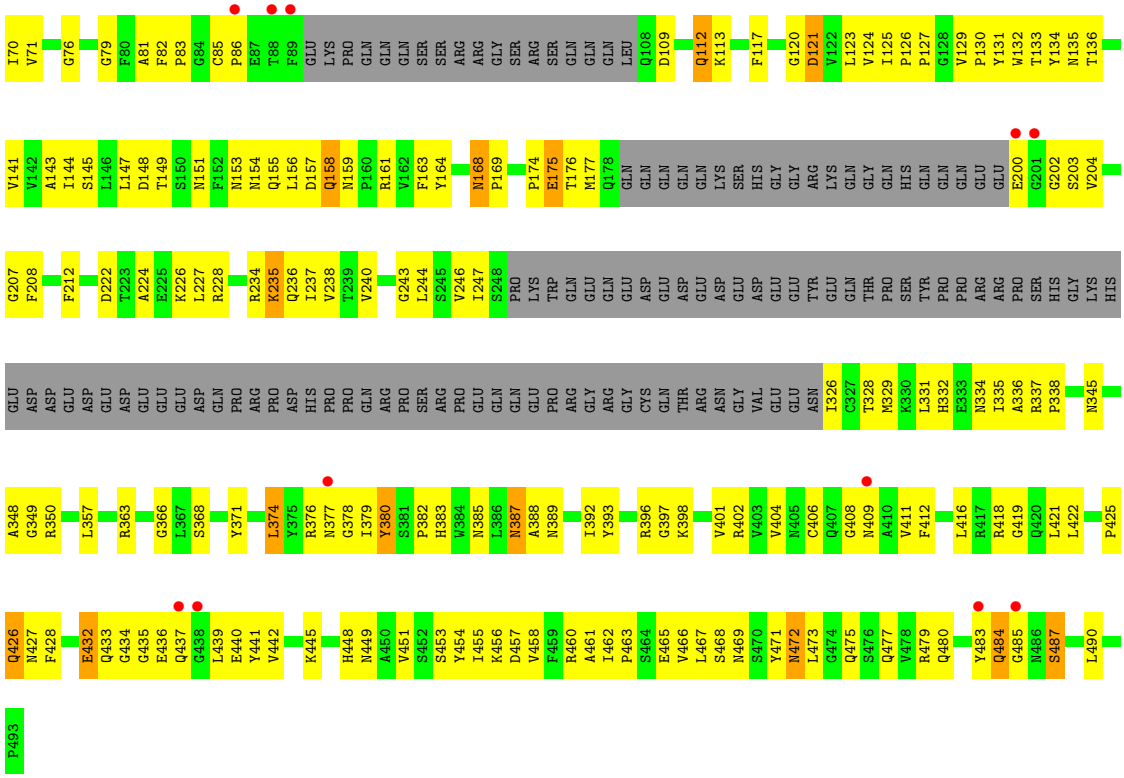


- Molecule 1: glycinin A3B4 subunit

Chain B:

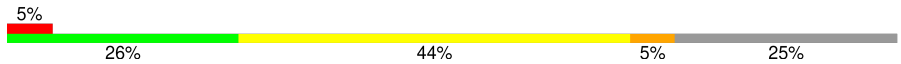


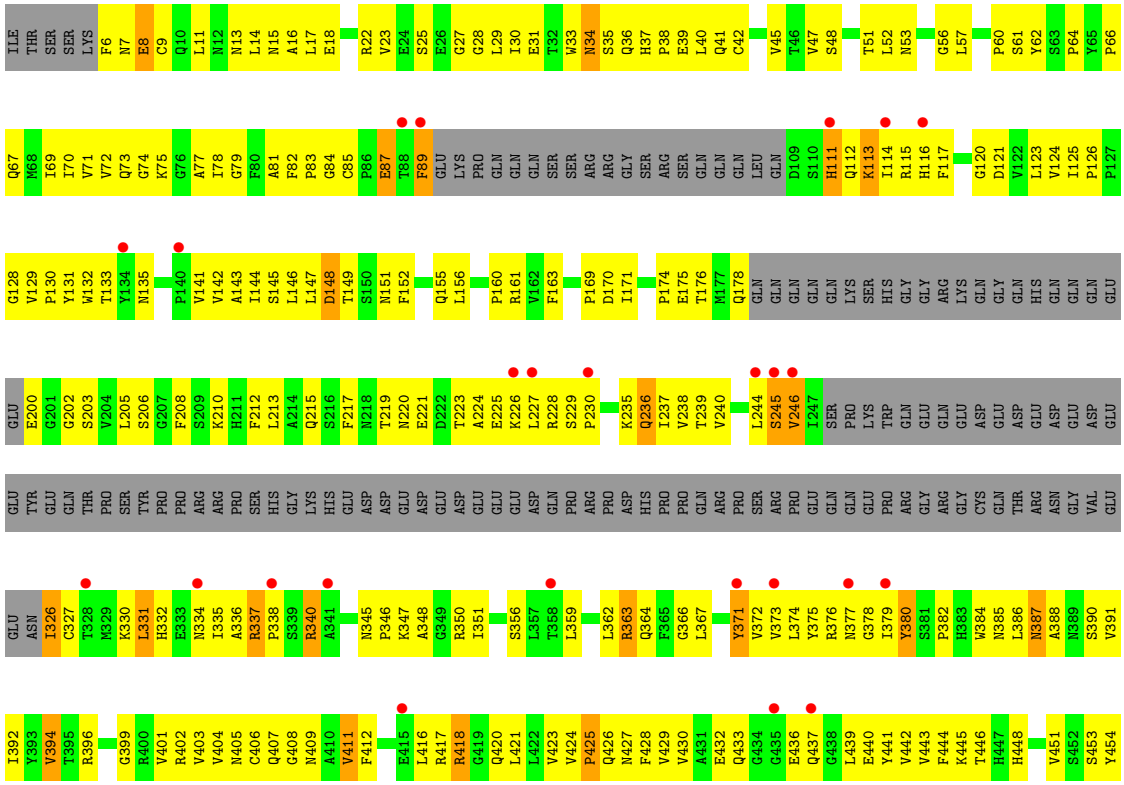


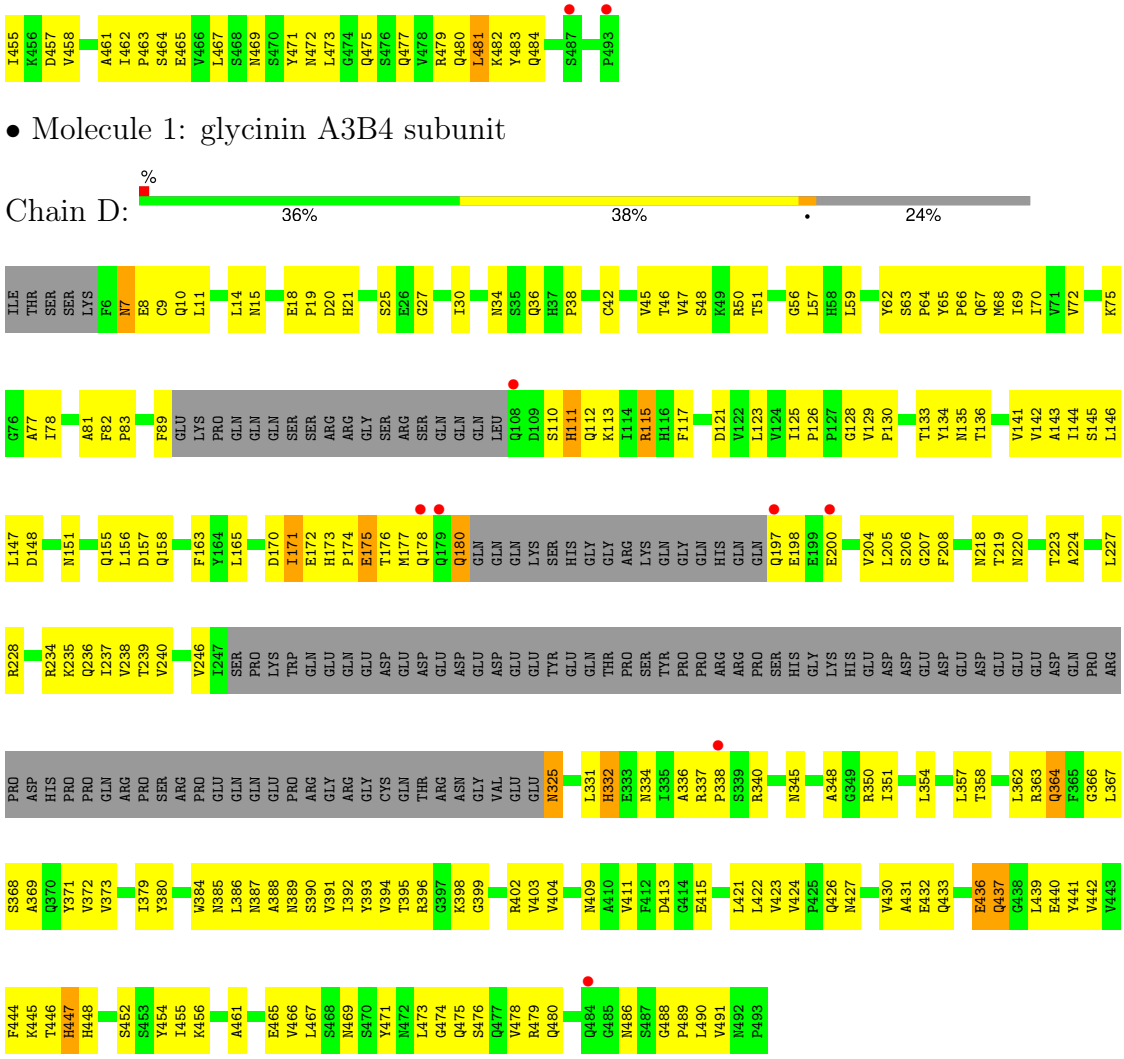


- Molecule 1: glycinin A3B4 subunit

Chain C:





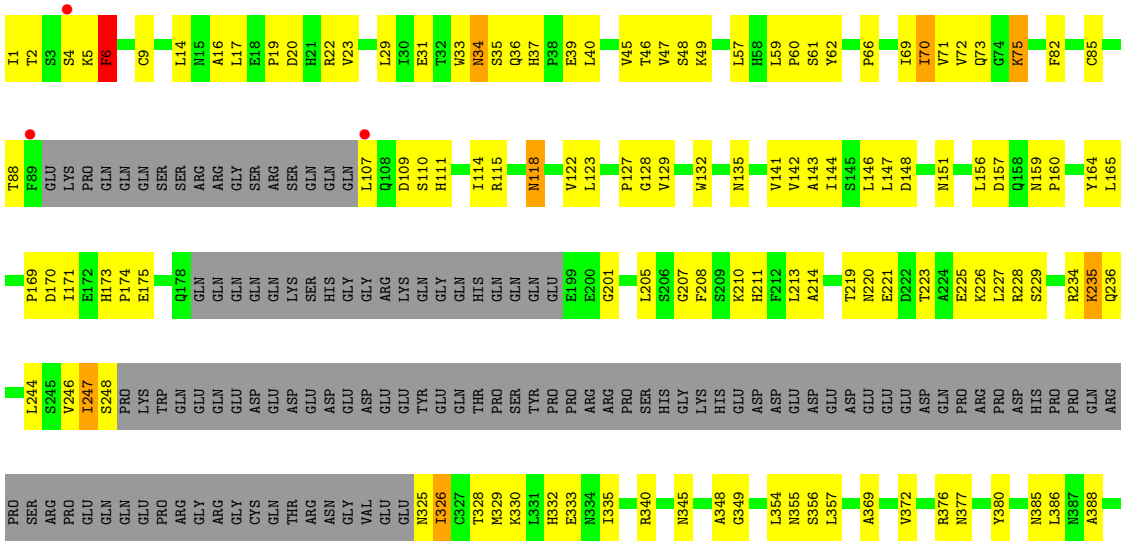


• Molecule 1: glycinin A3B4 subunit

Chain D:

• Molecule 1: glycinin A3B4 subunit

Chain E:

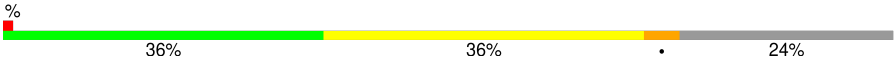


I392 Y393 V394 K398 V401 N405 C406 Q407 V411 E415 L416 R417 R418 G419 Q420 L421 P425 Q426 N427 F428 V429 V430 A431 E432 Y441 V442 V443 T446 H447 S452 S453 Y454 I455 K456 D457 V458 F459 R460 A461 I462 P463 S464 E465 V466 L467 S468 N469 S470 Y471 N472 L473

S476 Q477 V478 R479 Q480 L481 K482 Y483 Q484 G485 N486 S487 G488 P489 L490 V491 N492 P493

- Molecule 1: glycinin A3B4 subunit

Chain F:



ILE THR SER SER LYS F6 N7 L14 P19 D20 H21 S25 E26 G27 G28 L29 I30 E31 N34 S35 Q36 H37 P38 E39 L40 Q41 C42 V45 T46 K49 R50 T51 L52 N53 L59 P60 S61 Y62 Y65 P66 Q67 M68 I69 I70 V71 V72 G76 A77 I78 A81

F82 C85 P86 E87 T88 F89 E90 LYS PRO GLN GLN GLN GLN SER SER ARG ARG GLY SER ARG SER GLN GLN Q106 L107 Q108 D109 S110 H111 Q112 K113 I114 R115 H116 F117 N118 D121 V122 L123 V124 I125 P126 P127 G128 V129 P130 Y131 W132 T133 Y134 N135 T136 V141 I144 S145 L146 L147

D148 T149 S150 N151 F152 N153 N154 Q155 N159 P160 F163 Y164 G167 D170 I171 T176 Q179 GLN GLN GLN GLN LYS SER HIS GLY GLY ARG LYS GLN GLY GLN HIS GLN GLN GLN GLU GLU E200 S203 V204 L205 F208 F212 L213 A214 F217 N218 T219 N220 E221

D222 T223 A224 E225 K226 P230 D231 D232 E233 R234 K235 Q236 I237 V238 T239 V240 G243 L244 S245 V246 I247 S248 PRO LYS TRP GLN GLU GLN GLU ASP GLU ASP GLU ASP GLU ASP GLU GLU GLU TYR GLU GLN THR PRO SER TYR PRO PRO ARG ARG PRO SER HIS GLY LYS HIS GLU ASP ASP

GLU ASP GLU ASP GLU GLU GLU ASP GLN PRO ARG PRO ASP HIS PRO PRO GLN ARG PRO SER ARG PRO GLU GLN GLN GLU PRO ARG GLY ARG GLY CYS GLN THR ARG ASN GLY VAL GLU GLU N325 T328 M329 K330 L331 H332 E333 N334 I335 A336 R337 R340 F343 Y344 N345 A348

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

A431 E432 Q433 G434 G435 E436 L439 E440 Y441 K445 Y454 I455 K456 D457 V458 A461 I462 P463 S464 E465 V466 L467 S468 Y471 N472 L473 G474 Q477 V478 R479 Q480 L481 K482 Y483 N486 L490 V491 N492 P493

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.79 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.325 0.222 , 0.295	Depositor DCC
R_{free} test set	5961 reflections (9.43%)	wwPDB-VP
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 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
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
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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, CSD, CO3

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 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	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
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 35.

The worst 5 of 1233 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: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 (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	365/493 (74%)	302 (83%)	54 (15%)	9 (2%)	5 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	363/493 (74%)	297 (82%)	54 (15%)	12 (3%)	4	13
1	C	361/493 (73%)	291 (81%)	51 (14%)	19 (5%)	2	6
1	D	368/493 (75%)	307 (83%)	54 (15%)	7 (2%)	8	26
1	E	371/493 (75%)	311 (84%)	54 (15%)	6 (2%)	9	31
1	F	368/493 (75%)	311 (84%)	44 (12%)	13 (4%)	3	12
All	All	2196/2958 (74%)	1819 (83%)	311 (14%)	66 (3%)	4	15

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 (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	324/435 (74%)	310 (96%)	14 (4%)	29	62
1	B	322/435 (74%)	313 (97%)	9 (3%)	43	77
1	C	320/435 (74%)	305 (95%)	15 (5%)	26	59
1	D	327/435 (75%)	314 (96%)	13 (4%)	31	65
1	E	330/435 (76%)	318 (96%)	12 (4%)	35	69
1	F	327/435 (75%)	316 (97%)	11 (3%)	37	71
All	All	1950/2610 (75%)	1876 (96%)	74 (4%)	33	67

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

Mol	Chain	Res	Type
1	E	247	ILE

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Mol	Chain	Res	Type
1	F	332	HIS
1	E	380	TYR
1	F	65	TYR
1	C	87	GLU

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

Mol	Chain	Res	Type
1	F	67	GLN
1	F	179	GLN
1	F	437	GLN
1	B	472	ASN
1	B	449	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	D	406	1	4,7,8	0.60	0	1,8,10	1.36	0
1	CSD	F	406	1	4,7,8	0.61	0	1,8,10	1.37	0
1	CSD	E	406	1	4,7,8	0.56	0	1,8,10	1.16	0
1	CSD	B	406	1	4,7,8	0.62	0	1,8,10	1.41	0
1	CSD	C	406	1	4,7,8	0.59	0	1,8,10	0.75	0
1	CSD	A	406	1	4,7,8	0.60	0	1,8,10	0.98	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
1	CSD	D	406	1	-	0/2/6/8	-
1	CSD	F	406	1	-	1/2/6/8	-
1	CSD	E	406	1	-	1/2/6/8	-
1	CSD	B	406	1	-	1/2/6/8	-
1	CSD	C	406	1	-	1/2/6/8	-
1	CSD	A	406	1	-	0/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	406	CSD	CA-CB-SG-OD1
1	F	406	CSD	CA-CB-SG-OD1
1	B	406	CSD	CA-CB-SG-OD1
1	C	406	CSD	CA-CB-SG-OD1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	406	CSD	1	0
1	B	406	CSD	2	0
1	C	406	CSD	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	-	3,3,3	0.68	0	2,3,3	0.16	0
2	CO3	C	503	-	3,3,3	0.68	0	2,3,3	0.15	0
2	CO3	B	502	-	3,3,3	0.76	0	2,3,3	0.18	0
2	CO3	E	505	-	3,3,3	0.77	0	2,3,3	0.07	0
2	CO3	D	504	-	3,3,3	0.71	0	2,3,3	0.11	0
2	CO3	F	506	-	3,3,3	0.72	0	2,3,3	0.14	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	CO3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	373/493 (75%)	0.07	18 (4%)	30	21	13, 37, 54, 62	0
1	B	371/493 (75%)	0.01	12 (3%)	47	37	6, 37, 56, 63	0
1	C	369/493 (74%)	0.26	27 (7%)	15	8	7, 39, 54, 66	0
1	D	376/493 (76%)	-0.39	7 (1%)	66	59	6, 19, 46, 57	0
1	E	379/493 (76%)	-0.44	3 (0%)	86	81	6, 13, 43, 58	0
1	F	376/493 (76%)	-0.42	3 (0%)	86	81	6, 18, 45, 56	0
All	All	2244/2958 (75%)	-0.15	70 (3%)	49	39	6, 28, 52, 66	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	THR	6.0
1	B	437	GLN	4.7
1	C	89	PHE	4.4
1	C	435	GLY	4.4
1	C	226	LYS	3.7

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	CSD	C	406	8/9	0.88	0.16	31,38,58,62	0
1	CSD	A	406	8/9	0.91	0.16	30,41,46,53	0
1	CSD	B	406	8/9	0.94	0.14	39,44,63,73	0
1	CSD	F	406	8/9	0.95	0.17	5,8,30,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	E	406	8/9	0.96	0.14	5,7,45,53	0
1	CSD	D	406	8/9	0.96	0.10	5,13,23,38	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	CO3	F	506	4/4	0.87	0.19	5,5,18,21	0
2	CO3	B	502	4/4	0.88	0.22	12,22,39,45	0
2	CO3	A	501	4/4	0.88	0.24	14,35,39,41	0
2	CO3	E	505	4/4	0.89	0.17	5,5,10,17	0
2	CO3	C	503	4/4	0.91	0.16	36,40,41,42	0
3	MG	B	602	1/1	0.91	0.21	41,41,41,41	0
3	MG	C	603	1/1	0.93	0.13	21,21,21,21	0
3	MG	A	601	1/1	0.94	0.08	17,17,17,17	0
3	MG	D	604	1/1	0.96	0.16	17,17,17,17	0
2	CO3	D	504	4/4	0.97	0.14	5,19,20,21	0
3	MG	F	606	1/1	0.97	0.14	8,8,8,8	0
3	MG	E	605	1/1	0.99	0.16	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.