Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 04:00 AM EDT

PDB ID	:	7M6U
Title	:	Crystal structure of a circular permutation and computationally designed pro-enzyme of carboxypeptidase G2
Authors	:	Yachnin, B.J.; Khare, S.D.
Deposited on	:	2021-03-26
Resolution	:	2.59 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

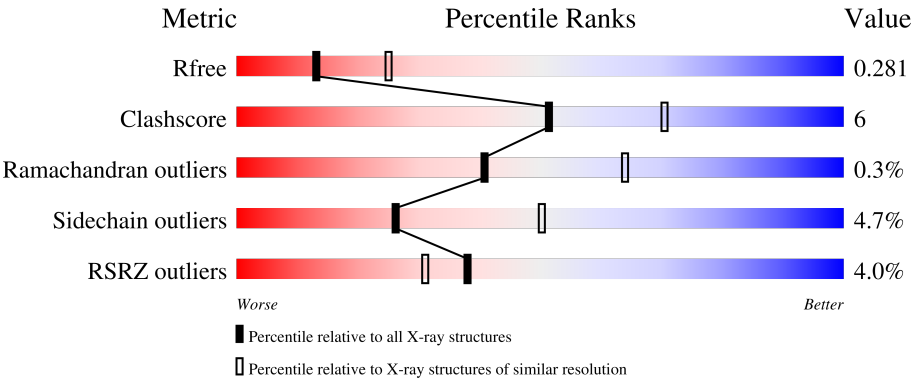
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	446	78% 9% • 12%
1	B	446	% 77% 10% • 12%
1	C	446	3% 78% 8% • 13%
1	D	446	10% 69% 10% • 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11105 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 Carboxypeptidase G2 circular permuation pro-domain fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2854	1793	491	564	6			
1	B	392	Total	C	N	O	S	0	0	0
			2849	1786	491	566	6			
1	C	389	Total	C	N	O	S	0	0	0
			2772	1731	477	558	6			
1	D	356	Total	C	N	O	S	0	0	0
			2473	1537	425	507	4			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP P06621
A	-24	GLY	-	expression tag	UNP P06621
A	-23	SER	-	expression tag	UNP P06621
A	-22	SER	-	expression tag	UNP P06621
A	-21	HIS	-	expression tag	UNP P06621
A	-20	HIS	-	expression tag	UNP P06621
A	-19	HIS	-	expression tag	UNP P06621
A	-18	HIS	-	expression tag	UNP P06621
A	-17	HIS	-	expression tag	UNP P06621
A	-16	HIS	-	expression tag	UNP P06621
A	-15	SER	-	expression tag	UNP P06621
A	-14	SER	-	expression tag	UNP P06621
A	-13	GLY	-	expression tag	UNP P06621
A	-12	LEU	-	expression tag	UNP P06621
A	-11	VAL	-	expression tag	UNP P06621
A	-10	PRO	-	expression tag	UNP P06621
A	-9	ARG	-	expression tag	UNP P06621
A	-8	GLY	-	expression tag	UNP P06621
A	-7	SER	-	expression tag	UNP P06621
A	-6	HIS	-	expression tag	UNP P06621
A	-5	MET	-	expression tag	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P06621
A	-3	SER	-	expression tag	UNP P06621
A	86	ALA	LYS	engineered mutation	UNP P06621
A	325	GLY	-	linker	UNP P06621
A	326	THR	-	linker	UNP P06621
A	327	ALA	-	linker	UNP P06621
A	328	SER	-	linker	UNP P06621
B	-25	MET	-	initiating methionine	UNP P06621
B	-24	GLY	-	expression tag	UNP P06621
B	-23	SER	-	expression tag	UNP P06621
B	-22	SER	-	expression tag	UNP P06621
B	-21	HIS	-	expression tag	UNP P06621
B	-20	HIS	-	expression tag	UNP P06621
B	-19	HIS	-	expression tag	UNP P06621
B	-18	HIS	-	expression tag	UNP P06621
B	-17	HIS	-	expression tag	UNP P06621
B	-16	HIS	-	expression tag	UNP P06621
B	-15	SER	-	expression tag	UNP P06621
B	-14	SER	-	expression tag	UNP P06621
B	-13	GLY	-	expression tag	UNP P06621
B	-12	LEU	-	expression tag	UNP P06621
B	-11	VAL	-	expression tag	UNP P06621
B	-10	PRO	-	expression tag	UNP P06621
B	-9	ARG	-	expression tag	UNP P06621
B	-8	GLY	-	expression tag	UNP P06621
B	-7	SER	-	expression tag	UNP P06621
B	-6	HIS	-	expression tag	UNP P06621
B	-5	MET	-	expression tag	UNP P06621
B	-4	GLY	-	expression tag	UNP P06621
B	-3	SER	-	expression tag	UNP P06621
B	86	ALA	LYS	engineered mutation	UNP P06621
B	325	GLY	-	linker	UNP P06621
B	326	THR	-	linker	UNP P06621
B	327	ALA	-	linker	UNP P06621
B	328	SER	-	linker	UNP P06621
C	-25	MET	-	initiating methionine	UNP P06621
C	-24	GLY	-	expression tag	UNP P06621
C	-23	SER	-	expression tag	UNP P06621
C	-22	SER	-	expression tag	UNP P06621
C	-21	HIS	-	expression tag	UNP P06621
C	-20	HIS	-	expression tag	UNP P06621
C	-19	HIS	-	expression tag	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP P06621
C	-17	HIS	-	expression tag	UNP P06621
C	-16	HIS	-	expression tag	UNP P06621
C	-15	SER	-	expression tag	UNP P06621
C	-14	SER	-	expression tag	UNP P06621
C	-13	GLY	-	expression tag	UNP P06621
C	-12	LEU	-	expression tag	UNP P06621
C	-11	VAL	-	expression tag	UNP P06621
C	-10	PRO	-	expression tag	UNP P06621
C	-9	ARG	-	expression tag	UNP P06621
C	-8	GLY	-	expression tag	UNP P06621
C	-7	SER	-	expression tag	UNP P06621
C	-6	HIS	-	expression tag	UNP P06621
C	-5	MET	-	expression tag	UNP P06621
C	-4	GLY	-	expression tag	UNP P06621
C	-3	SER	-	expression tag	UNP P06621
C	86	ALA	LYS	engineered mutation	UNP P06621
C	325	GLY	-	linker	UNP P06621
C	326	THR	-	linker	UNP P06621
C	327	ALA	-	linker	UNP P06621
C	328	SER	-	linker	UNP P06621
D	-25	MET	-	initiating methionine	UNP P06621
D	-24	GLY	-	expression tag	UNP P06621
D	-23	SER	-	expression tag	UNP P06621
D	-22	SER	-	expression tag	UNP P06621
D	-21	HIS	-	expression tag	UNP P06621
D	-20	HIS	-	expression tag	UNP P06621
D	-19	HIS	-	expression tag	UNP P06621
D	-18	HIS	-	expression tag	UNP P06621
D	-17	HIS	-	expression tag	UNP P06621
D	-16	HIS	-	expression tag	UNP P06621
D	-15	SER	-	expression tag	UNP P06621
D	-14	SER	-	expression tag	UNP P06621
D	-13	GLY	-	expression tag	UNP P06621
D	-12	LEU	-	expression tag	UNP P06621
D	-11	VAL	-	expression tag	UNP P06621
D	-10	PRO	-	expression tag	UNP P06621
D	-9	ARG	-	expression tag	UNP P06621
D	-8	GLY	-	expression tag	UNP P06621
D	-7	SER	-	expression tag	UNP P06621
D	-6	HIS	-	expression tag	UNP P06621
D	-5	MET	-	expression tag	UNP P06621

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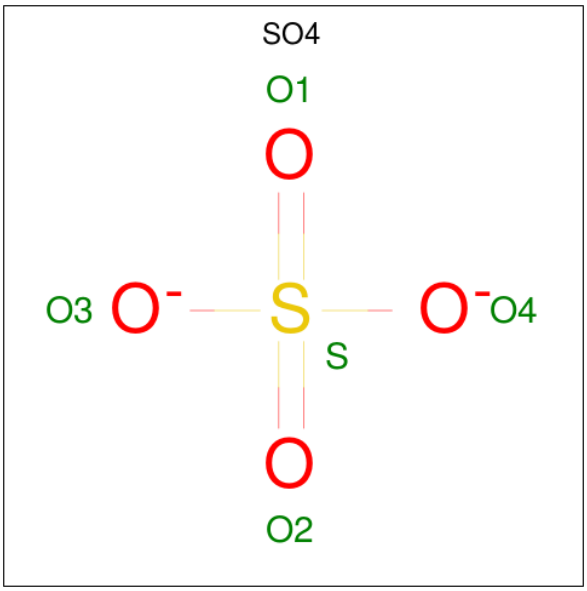
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP P06621
D	-3	SER	-	expression tag	UNP P06621
D	86	ALA	LYS	engineered mutation	UNP P06621
D	325	GLY	-	linker	UNP P06621
D	326	THR	-	linker	UNP P06621
D	327	ALA	-	linker	UNP P06621
D	328	SER	-	linker	UNP P06621

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total Zn 7 7	0	0
2	B	5	Total Zn 5 5	0	0
2	C	4	Total Zn 4 4	0	0
2	D	4	Total Zn 4 4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

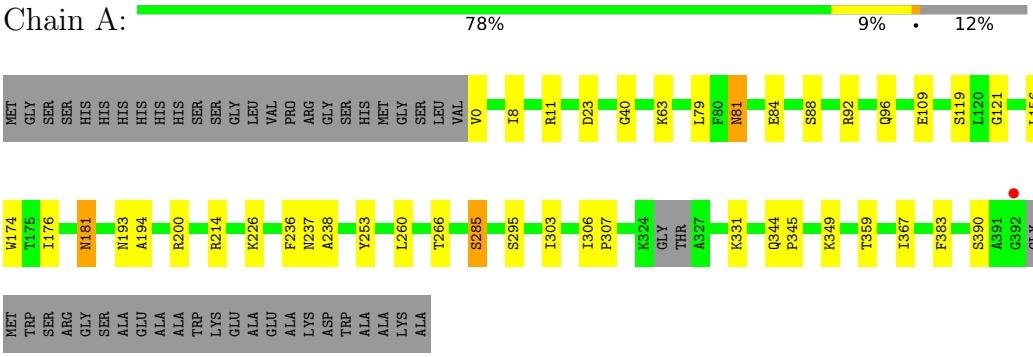
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	54	Total O 54 54	0	0
4	B	43	Total O 43 43	0	0
4	C	22	Total O 22 22	0	0
4	D	13	Total O 13 13	0	0

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.

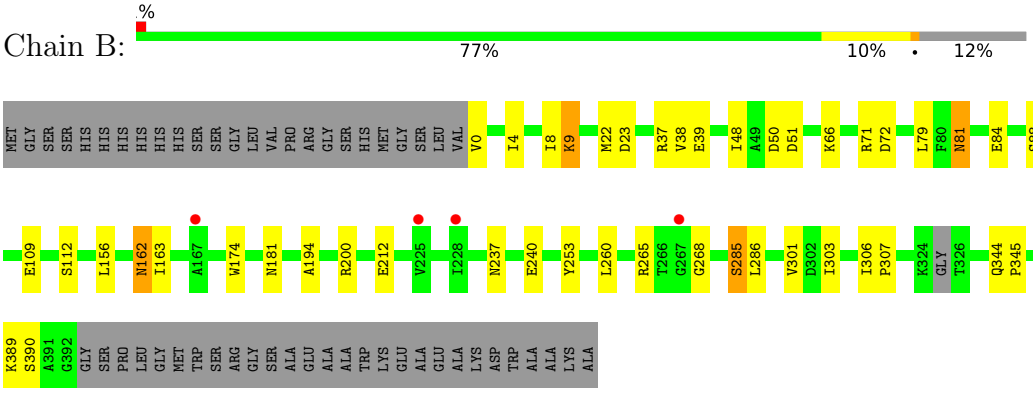
• Molecule 1: Carboxypeptidase G2 circular permuation pro-domain fusion

Chain A:



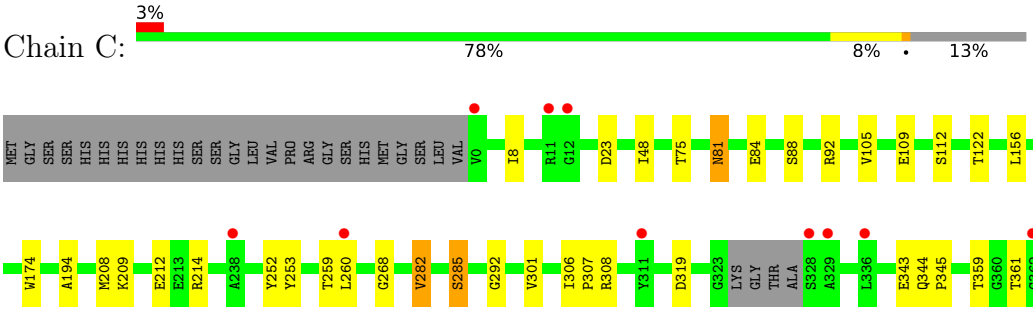
• Molecule 1: Carboxypeptidase G2 circular permuation pro-domain fusion

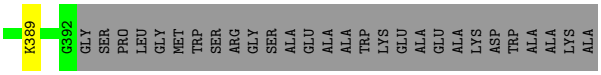
Chain B:



• Molecule 1: Carboxypeptidase G2 circular permuation pro-domain fusion

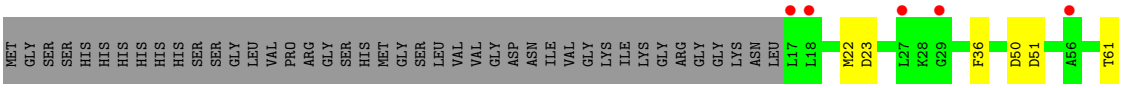
Chain C:

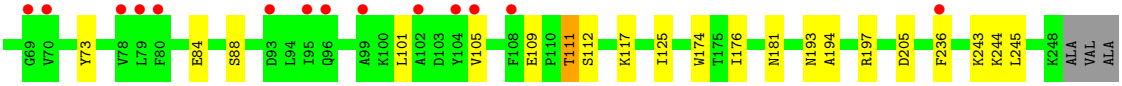


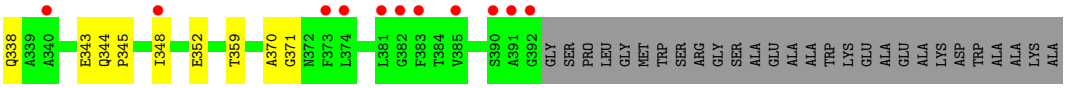


• Molecule 1: Carboxypeptidase G2 circular permuation pro-domain fusion

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.54Å 106.36Å 121.93Å 90.00° 107.48° 90.00°	Depositor
Resolution (Å)	39.27 – 2.59 39.24 – 2.59	Depositor EDS
% Data completeness (in resolution range)	80.9 (39.27-2.59) 81.0 (39.24-2.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.222 , 0.279 0.225 , 0.281	Depositor DCC
R_{free} test set	2346 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11105	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.72	0/2893	0.83	0/3917
1	B	0.69	0/2887	0.82	0/3913
1	C	0.70	0/2811	0.83	0/3820
1	D	0.73	0/2506	0.83	0/3415
All	All	0.71	0/11097	0.83	0/15065

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

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	2854	0	2813	27	0
1	B	2849	0	2782	28	0
1	C	2772	0	2609	26	0
1	D	2473	0	2240	40	0
2	A	7	0	0	0	0
2	B	5	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	54	0	0	2	0
4	B	43	0	0	2	0
4	C	22	0	0	1	0
4	D	13	0	0	1	0
All	All	11105	0	10444	120	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 6.

All (120) 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:244:LYS:HE2	1:D:315:ARG:HG2	1.43	0.99
1:D:334:ASN:O	1:D:338:GLN:HG2	1.79	0.82
1:B:81:ASN:HD22	1:B:81:ASN:H	1.30	0.80
1:A:81:ASN:H	1:A:81:ASN:HD22	1.29	0.79
1:C:81:ASN:HD22	1:C:81:ASN:H	1.30	0.78
1:A:162:ASN:C	1:A:162:ASN:HD22	1.85	0.77
1:D:315:ARG:O	1:D:315:ARG:CZ	2.32	0.77
1:D:315:ARG:O	1:D:315:ARG:NH1	2.18	0.77
1:C:105:VAL:HB	1:C:282:VAL:HG12	1.68	0.74
1:C:105:VAL:HB	1:C:282:VAL:CG1	2.17	0.74
1:D:111:THR:HG21	1:D:117:LYS:O	1.91	0.71
1:B:162:ASN:C	1:B:162:ASN:HD22	1.92	0.71
1:C:208:MET:O	1:C:212:GLU:HG2	1.89	0.71
1:C:162:ASN:HD22	1:C:162:ASN:C	1.96	0.68
1:D:333:ASP:OD1	1:D:335:VAL:CG2	2.42	0.67
1:D:303:ILE:HD11	1:D:348:ILE:HG12	1.76	0.66
1:D:105:VAL:CB	1:D:282:VAL:HG12	2.29	0.62
1:D:125:ILE:HD12	1:D:197:ARG:NH1	2.15	0.61
1:D:61:THR:HG21	1:D:313:ALA:HA	1.82	0.61
1:B:39:GLU:HA	4:B:624:HOH:O	2.02	0.60
1:D:333:ASP:OD1	1:D:335:VAL:HG23	2.01	0.60
1:A:109:GLU:O	1:A:285:SER:HA	2.04	0.57
1:D:333:ASP:OD1	1:D:335:VAL:HG22	2.03	0.57
1:C:109:GLU:O	1:C:285:SER:HA	2.04	0.57
1:B:162:ASN:C	1:B:162:ASN:ND2	2.58	0.57
1:C:81:ASN:HD22	1:C:81:ASN:N	2.00	0.56
1:D:109:GLU:O	1:D:285:SER:HA	2.06	0.56
1:C:162:ASN:C	1:C:162:ASN:ND2	2.58	0.56
1:A:162:ASN:C	1:A:162:ASN:ND2	2.58	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:O	1:B:285:SER:HA	2.06	0.54
1:A:162:ASN:HD21	1:A:214:ARG:HH22	1.56	0.54
1:C:252:TYR:OH	1:C:319:ASP:OD2	2.26	0.54
1:B:162:ASN:HD22	1:B:163:ILE:N	2.07	0.53
1:B:268:GLY:HA2	4:B:617:HOH:O	2.07	0.53
1:A:162:ASN:HD22	1:A:163:ILE:N	2.08	0.52
1:C:162:ASN:HD21	1:C:214:ARG:NH2	2.08	0.51
1:A:200:ARG:HD2	1:A:237:ASN:ND2	2.26	0.51
1:A:236:PHE:HA	4:A:604:HOH:O	2.10	0.51
1:B:0:VAL:HB	1:B:390:SER:HB2	1.93	0.51
1:B:9:LYS:O	1:B:71:ARG:NH1	2.43	0.51
1:B:240:GLU:H	1:B:240:GLU:CD	2.13	0.51
1:B:84:GLU:HA	1:B:88:SER:OG	2.11	0.51
1:B:81:ASN:HD22	1:B:81:ASN:N	2.01	0.51
1:C:84:GLU:HA	1:C:88:SER:OG	2.11	0.50
1:D:111:THR:HG21	1:D:117:LYS:H	1.74	0.50
1:A:174:TRP:CE3	1:A:194:ALA:HB2	2.46	0.50
1:D:84:GLU:HA	1:D:88:SER:OG	2.10	0.50
1:A:119:SER:HB2	1:A:266:THR:HG22	1.92	0.50
1:A:84:GLU:HA	1:A:88:SER:OG	2.11	0.50
1:A:200:ARG:HH11	1:A:237:ASN:HD22	1.60	0.50
1:A:181:ASN:ND2	1:B:181:ASN:OD1	2.43	0.49
1:C:162:ASN:HD22	1:C:163:ILE:N	2.10	0.49
1:C:174:TRP:CE3	1:C:194:ALA:HB2	2.48	0.49
1:A:253:TYR:CD2	1:A:260:LEU:HG	2.48	0.49
1:C:253:TYR:CD2	1:C:260:LEU:HG	2.48	0.49
1:D:174:TRP:CE3	1:D:194:ALA:HB2	2.48	0.48
1:B:174:TRP:CE3	1:B:194:ALA:HB2	2.48	0.48
1:C:105:VAL:HB	1:C:282:VAL:HG13	1.92	0.48
1:C:253:TYR:CZ	1:C:308:ARG:HD2	2.47	0.48
1:B:253:TYR:CD2	1:B:260:LEU:HG	2.49	0.48
1:A:8:ILE:HG22	1:A:383:PHE:CE2	2.49	0.48
1:A:306:ILE:HB	1:A:307:PRO:HD3	1.95	0.48
1:C:306:ILE:HB	1:C:307:PRO:HD3	1.95	0.48
1:A:344:GLN:HB3	1:A:345:PRO:HD3	1.96	0.47
1:B:306:ILE:HB	1:B:307:PRO:HD3	1.96	0.47
1:C:8:ILE:HG22	1:C:383:PHE:CE2	2.49	0.47
1:D:244:LYS:NZ	1:D:312:MET:O	2.48	0.47
1:A:81:ASN:HD22	1:A:81:ASN:N	2.00	0.47
1:A:359:THR:HB	1:A:367:ILE:HD13	1.96	0.47
1:B:8:ILE:HG22	1:B:383:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:MET:HE1	1:D:371:GLY:N	2.30	0.47
1:B:4:ILE:HG12	1:B:22:MET:HE1	1.96	0.47
1:B:38:VAL:HG23	1:B:303:ILE:HD11	1.97	0.47
1:D:22:MET:HE1	1:D:370:ALA:CB	2.45	0.47
1:D:125:ILE:CD1	1:D:197:ARG:NH1	2.78	0.47
1:D:244:LYS:CE	1:D:312:MET:O	2.63	0.46
1:D:344:GLN:HB3	1:D:345:PRO:HD3	1.97	0.46
1:D:306:ILE:HB	1:D:307:PRO:HD3	1.97	0.46
1:D:36:PHE:CD2	1:D:352:GLU:HA	2.50	0.46
1:C:292:GLY:O	4:C:601:HOH:O	2.21	0.46
1:B:38:VAL:HG23	1:B:303:ILE:CD1	2.46	0.46
1:C:260:LEU:HD23	1:C:260:LEU:HA	1.83	0.46
1:D:284:GLU:HA	1:D:284:GLU:OE1	2.16	0.45
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.60	0.45
1:D:236:PHE:HE1	1:D:282:VAL:HG23	1.80	0.45
1:C:162:ASN:HD21	1:C:214:ARG:HH22	1.64	0.45
1:C:122:THR:HB	1:C:268:GLY:O	2.17	0.44
1:B:344:GLN:HB3	1:B:345:PRO:HD3	1.98	0.44
1:D:111:THR:CG2	1:D:117:LYS:O	2.64	0.44
1:D:244:LYS:HE3	1:D:312:MET:O	2.19	0.43
1:C:344:GLN:HB3	1:C:345:PRO:HD3	2.00	0.43
1:D:295:SER:O	4:D:601:HOH:O	2.21	0.43
1:A:23:ASP:HA	1:A:359:THR:O	2.19	0.43
1:C:23:ASP:HA	1:C:359:THR:O	2.19	0.43
1:D:284:GLU:OE1	1:D:285:SER:N	2.44	0.43
1:A:92:ARG:O	1:A:96:GLN:HG3	2.19	0.42
1:D:109:GLU:HG3	1:D:284:GLU:OE2	2.20	0.42
1:B:200:ARG:HD2	1:B:237:ASN:ND2	2.34	0.42
1:D:23:ASP:HA	1:D:359:THR:O	2.20	0.42
1:A:40:GLY:O	1:A:303:ILE:HD11	2.19	0.42
1:D:343:GLU:OE2	1:D:343:GLU:HA	2.19	0.42
1:A:119:SER:OG	1:A:121:GLY:O	2.37	0.42
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.85	0.41
1:B:48:ILE:HG23	1:B:301:VAL:HG13	2.02	0.41
1:B:50:ASP:HA	1:B:51:ASP:HA	1.83	0.41
1:C:343:GLU:OE2	1:C:343:GLU:HA	2.20	0.41
1:D:109:GLU:CG	1:D:284:GLU:OE2	2.69	0.41
1:B:260:LEU:HD23	1:B:260:LEU:HA	1.84	0.41
1:A:0:VAL:HB	1:A:390:SER:HB2	2.01	0.41
1:B:92:ARG:O	1:B:96:GLN:HG3	2.20	0.41
1:D:176:ILE:HB	1:D:193:ASN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HB	1:A:193:ASN:HB2	2.03	0.41
1:B:23:ASP:HA	1:B:359:THR:O	2.21	0.41
1:D:22:MET:CE	1:D:370:ALA:C	2.89	0.41
1:C:48:ILE:HG23	1:C:301:VAL:HG13	2.02	0.40
1:D:236:PHE:HE1	1:D:282:VAL:CG2	2.34	0.40
1:D:22:MET:HE1	1:D:370:ALA:C	2.41	0.40
1:D:50:ASP:HA	1:D:51:ASP:HA	1.82	0.40
1:A:238:ALA:N	4:A:602:HOH:O	2.55	0.40
1:D:284:GLU:OE1	1:D:284:GLU:CA	2.70	0.40

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	387/446 (87%)	370 (96%)	15 (4%)	2 (0%)	29	52
1	B	388/446 (87%)	375 (97%)	12 (3%)	1 (0%)	41	64
1	C	385/446 (86%)	370 (96%)	14 (4%)	1 (0%)	41	64
1	D	350/446 (78%)	329 (94%)	20 (6%)	1 (0%)	41	64
All	All	1510/1784 (85%)	1444 (96%)	61 (4%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	SER
1	C	285	SER
1	A	285	SER
1	A	331	LYS
1	D	285	SER

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	279/334 (84%)	269 (96%)	10 (4%)	35	61
1	B	276/334 (83%)	262 (95%)	14 (5%)	24	46
1	C	256/334 (77%)	245 (96%)	11 (4%)	29	54
1	D	219/334 (66%)	206 (94%)	13 (6%)	19	39
All	All	1030/1336 (77%)	982 (95%)	48 (5%)	26	50

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	63	LYS
1	A	79	LEU
1	A	81	ASN
1	A	156	LEU
1	A	162	ASN
1	A	181	ASN
1	A	226	LYS
1	A	295	SER
1	A	349	LYS
1	B	9	LYS
1	B	37	ARG
1	B	66	LYS
1	B	72	ASP
1	B	79	LEU
1	B	81	ASN
1	B	92	ARG
1	B	112	SER
1	B	156	LEU
1	B	162	ASN
1	B	212	GLU
1	B	265	ARG
1	B	286	LEU
1	B	389	LYS

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Mol	Chain	Res	Type
1	C	75	THR
1	C	81	ASN
1	C	92	ARG
1	C	112	SER
1	C	156	LEU
1	C	162	ASN
1	C	209	LYS
1	C	259	THR
1	C	282	VAL
1	C	361	THR
1	C	389	LYS
1	D	73	TYR
1	D	101	LEU
1	D	111	THR
1	D	112	SER
1	D	181	ASN
1	D	205	ASP
1	D	243	LYS
1	D	245	LEU
1	D	264	GLU
1	D	282	VAL
1	D	284	GLU
1	D	295	SER
1	D	315	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	162	ASN
1	A	237	ASN
1	B	55	ASN
1	B	81	ASN
1	B	96	GLN
1	B	162	ASN
1	B	193	ASN
1	B	380	ASN
1	C	81	ASN
1	C	162	ASN
1	C	193	ASN
1	C	237	ASN
1	D	181	ASN

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Mol	Chain	Res	Type
1	D	193	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 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	SO4	A	507	-	4,4,4	0.32	0	6,6,6	0.10	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.

No monomer is involved in short contacts.

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, 95^{th} 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	391/446 (87%)	-0.23	1 (0%) 94 93	30, 44, 65, 110	0
1	B	392/446 (87%)	-0.21	4 (1%) 82 80	33, 50, 74, 102	0
1	C	389/446 (87%)	0.14	12 (3%) 49 42	31, 70, 95, 138	0
1	D	356/446 (79%)	0.50	44 (12%) 4 2	31, 78, 111, 137	0
All	All	1528/1784 (85%)	0.04	61 (3%) 38 31	30, 55, 99, 138	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	260	LEU	6.3
1	D	383	PHE	5.6
1	D	17	LEU	5.6
1	C	11	ARG	5.2
1	D	78	VAL	4.9
1	D	104	TYR	4.7
1	A	392	GLY	4.4
1	D	374	LEU	4.0
1	D	381	LEU	3.9
1	C	311	TYR	3.9
1	D	236	PHE	3.9
1	D	261	GLY	3.9
1	D	318	MET	3.9
1	C	364	ALA	3.8
1	D	382	GLY	3.7
1	D	99	ALA	3.7
1	D	391	ALA	3.5
1	D	95	ILE	3.5
1	D	79	LEU	3.4
1	C	12	GLY	3.4
1	C	336	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	80	PHE	3.2
1	D	277	LEU	3.2
1	C	328	SER	3.2
1	C	329	ALA	3.1
1	B	267	GLY	3.1
1	D	348	ILE	3.0
1	C	0	VAL	2.8
1	D	329	ALA	2.8
1	D	275	ALA	2.8
1	D	29	GLY	2.7
1	C	238	ALA	2.7
1	C	362	GLY	2.7
1	D	274	TYR	2.6
1	D	96	GLN	2.6
1	D	27	LEU	2.6
1	D	69	GLY	2.6
1	D	282	VAL	2.6
1	D	102	ALA	2.5
1	D	262	VAL	2.5
1	B	228	ILE	2.5
1	D	373	PHE	2.5
1	D	56	ALA	2.5
1	D	273	ALA	2.5
1	D	311	TYR	2.4
1	D	279	GLY	2.4
1	D	70	VAL	2.3
1	D	281	PRO	2.3
1	D	291	PHE	2.3
1	B	225	VAL	2.3
1	D	340	ALA	2.3
1	D	105	VAL	2.3
1	D	385	VAL	2.3
1	C	260	LEU	2.2
1	B	167	ALA	2.2
1	D	392	GLY	2.2
1	D	390	SER	2.2
1	C	170	LEU	2.1
1	D	93	ASP	2.1
1	D	18	LEU	2.1
1	D	108	PHE	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 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, 95^{th} 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	ZN	A	506	1/1	0.80	0.08	129,129,129,129	0
2	ZN	B	504	1/1	0.83	0.07	118,118,118,118	0
2	ZN	A	505	1/1	0.89	0.14	121,121,121,121	0
3	SO4	A	507	5/5	0.90	0.15	100,106,110,113	0
2	ZN	C	501	1/1	0.98	0.14	61,61,61,61	0
2	ZN	C	503	1/1	0.98	0.02	89,89,89,89	0
2	ZN	D	501	1/1	0.98	0.06	63,63,63,63	0
2	ZN	D	503	1/1	0.98	0.02	93,93,93,93	0
2	ZN	A	504	1/1	0.98	0.02	85,85,85,85	0
2	ZN	B	503	1/1	0.99	0.05	88,88,88,88	0
2	ZN	D	500	1/1	0.99	0.07	64,64,64,64	0
2	ZN	A	502	1/1	0.99	0.09	43,43,43,43	0
2	ZN	D	502	1/1	0.99	0.10	42,42,42,42	0
2	ZN	C	500	1/1	0.99	0.14	53,53,53,53	0
2	ZN	B	502	1/1	0.99	0.12	57,57,57,57	0
2	ZN	A	501	1/1	1.00	0.13	33,33,33,33	0
2	ZN	A	500	1/1	1.00	0.14	33,33,33,33	0
2	ZN	A	503	1/1	1.00	0.10	49,49,49,49	0
2	ZN	B	500	1/1	1.00	0.10	38,38,38,38	0
2	ZN	B	501	1/1	1.00	0.10	38,38,38,38	0
2	ZN	C	502	1/1	1.00	0.09	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.