Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 10:03 AM EST

PDB ID	:	6XJ5
Title	:	Carboxypeptidase G2 modified with a versatile bioconjugate for metalloprotein design
Authors	:	Yachnin, B.J.; Hansen, W.A.; Khare, S.D.
Deposited on	:	2020-06-22
Resolution	:	3.11 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:

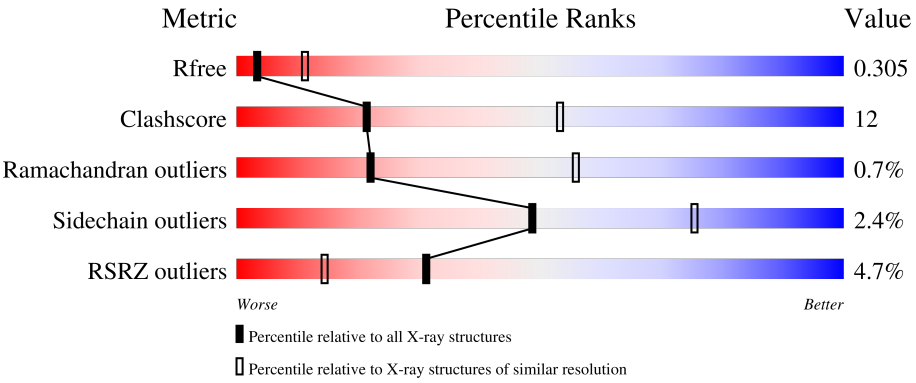
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	411	4% 78% 17% 5%
1	C	411	4% 73% 21% • 5%
1	E	411	5% 70% 23% • 5%
1	G	411	5% 76% 18% 6%
2	B	411	3% 76% 18% • 5%

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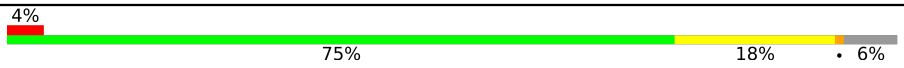
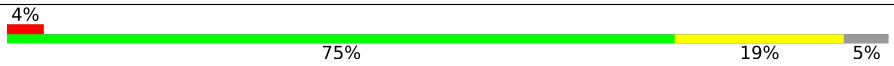
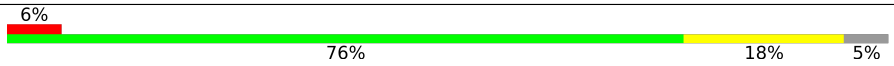
Mol	Chain	Length	Quality of chain
2	D	411	
2	F	411	
2	H	411	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21541 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2703	1700	464	532	7			
1	C	389	Total	C	N	O	S	0	0	0
			2671	1686	458	520	7			
1	E	389	Total	C	N	O	S	0	0	0
			2654	1665	453	531	5			
1	G	387	Total	C	N	O	S	0	0	0
			2648	1667	451	523	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	initiating methionine	UNP P06621
A	6	GLY	-	expression tag	UNP P06621
A	7	SER	-	expression tag	UNP P06621
A	8	ASP	-	expression tag	UNP P06621
A	9	LYS	-	expression tag	UNP P06621
A	10	ILE	-	expression tag	UNP P06621
A	11	HIS	-	expression tag	UNP P06621
A	12	HIS	-	expression tag	UNP P06621
A	13	HIS	-	expression tag	UNP P06621
A	14	HIS	-	expression tag	UNP P06621
A	15	HIS	-	expression tag	UNP P06621
A	16	HIS	-	expression tag	UNP P06621
A	17	GLU	-	expression tag	UNP P06621
A	18	ASN	-	expression tag	UNP P06621
A	19	LEU	-	expression tag	UNP P06621
A	20	TYR	-	expression tag	UNP P06621
A	21	PHE	-	expression tag	UNP P06621
A	22	GLN	-	expression tag	UNP P06621
A	23	GLY	-	expression tag	UNP P06621
A	203	CYS	SER	engineered mutation	UNP P06621
C	5	MET	-	initiating methionine	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLY	-	expression tag	UNP P06621
C	7	SER	-	expression tag	UNP P06621
C	8	ASP	-	expression tag	UNP P06621
C	9	LYS	-	expression tag	UNP P06621
C	10	ILE	-	expression tag	UNP P06621
C	11	HIS	-	expression tag	UNP P06621
C	12	HIS	-	expression tag	UNP P06621
C	13	HIS	-	expression tag	UNP P06621
C	14	HIS	-	expression tag	UNP P06621
C	15	HIS	-	expression tag	UNP P06621
C	16	HIS	-	expression tag	UNP P06621
C	17	GLU	-	expression tag	UNP P06621
C	18	ASN	-	expression tag	UNP P06621
C	19	LEU	-	expression tag	UNP P06621
C	20	TYR	-	expression tag	UNP P06621
C	21	PHE	-	expression tag	UNP P06621
C	22	GLN	-	expression tag	UNP P06621
C	23	GLY	-	expression tag	UNP P06621
C	203	CYS	SER	engineered mutation	UNP P06621
E	5	MET	-	initiating methionine	UNP P06621
E	6	GLY	-	expression tag	UNP P06621
E	7	SER	-	expression tag	UNP P06621
E	8	ASP	-	expression tag	UNP P06621
E	9	LYS	-	expression tag	UNP P06621
E	10	ILE	-	expression tag	UNP P06621
E	11	HIS	-	expression tag	UNP P06621
E	12	HIS	-	expression tag	UNP P06621
E	13	HIS	-	expression tag	UNP P06621
E	14	HIS	-	expression tag	UNP P06621
E	15	HIS	-	expression tag	UNP P06621
E	16	HIS	-	expression tag	UNP P06621
E	17	GLU	-	expression tag	UNP P06621
E	18	ASN	-	expression tag	UNP P06621
E	19	LEU	-	expression tag	UNP P06621
E	20	TYR	-	expression tag	UNP P06621
E	21	PHE	-	expression tag	UNP P06621
E	22	GLN	-	expression tag	UNP P06621
E	23	GLY	-	expression tag	UNP P06621
E	203	CYS	SER	engineered mutation	UNP P06621
G	5	MET	-	initiating methionine	UNP P06621
G	6	GLY	-	expression tag	UNP P06621
G	7	SER	-	expression tag	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
G	8	ASP	-	expression tag	UNP P06621
G	9	LYS	-	expression tag	UNP P06621
G	10	ILE	-	expression tag	UNP P06621
G	11	HIS	-	expression tag	UNP P06621
G	12	HIS	-	expression tag	UNP P06621
G	13	HIS	-	expression tag	UNP P06621
G	14	HIS	-	expression tag	UNP P06621
G	15	HIS	-	expression tag	UNP P06621
G	16	HIS	-	expression tag	UNP P06621
G	17	GLU	-	expression tag	UNP P06621
G	18	ASN	-	expression tag	UNP P06621
G	19	LEU	-	expression tag	UNP P06621
G	20	TYR	-	expression tag	UNP P06621
G	21	PHE	-	expression tag	UNP P06621
G	22	GLN	-	expression tag	UNP P06621
G	23	GLY	-	expression tag	UNP P06621
G	203	CYS	SER	engineered mutation	UNP P06621

- Molecule 2 is a protein called Carboxypeptidase G2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	0	0
			2692	1693	456	537	6			
2	D	386	Total	C	N	O	S	0	0	0
			2642	1661	453	523	5			
2	F	389	Total	C	N	O	S	0	0	0
			2635	1657	456	517	5			
2	H	389	Total	C	N	O	S	0	0	0
			2710	1703	471	530	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	MET	-	initiating methionine	UNP P06621
B	6	GLY	-	expression tag	UNP P06621
B	7	SER	-	expression tag	UNP P06621
B	8	ASP	-	expression tag	UNP P06621
B	9	LYS	-	expression tag	UNP P06621
B	10	ILE	-	expression tag	UNP P06621
B	11	HIS	-	expression tag	UNP P06621
B	12	HIS	-	expression tag	UNP P06621
B	13	HIS	-	expression tag	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	HIS	-	expression tag	UNP P06621
B	15	HIS	-	expression tag	UNP P06621
B	16	HIS	-	expression tag	UNP P06621
B	17	GLU	-	expression tag	UNP P06621
B	18	ASN	-	expression tag	UNP P06621
B	19	LEU	-	expression tag	UNP P06621
B	20	TYR	-	expression tag	UNP P06621
B	21	PHE	-	expression tag	UNP P06621
B	22	GLN	-	expression tag	UNP P06621
B	23	GLY	-	expression tag	UNP P06621
B	203	V44	SER	engineered mutation	UNP P06621
D	5	MET	-	initiating methionine	UNP P06621
D	6	GLY	-	expression tag	UNP P06621
D	7	SER	-	expression tag	UNP P06621
D	8	ASP	-	expression tag	UNP P06621
D	9	LYS	-	expression tag	UNP P06621
D	10	ILE	-	expression tag	UNP P06621
D	11	HIS	-	expression tag	UNP P06621
D	12	HIS	-	expression tag	UNP P06621
D	13	HIS	-	expression tag	UNP P06621
D	14	HIS	-	expression tag	UNP P06621
D	15	HIS	-	expression tag	UNP P06621
D	16	HIS	-	expression tag	UNP P06621
D	17	GLU	-	expression tag	UNP P06621
D	18	ASN	-	expression tag	UNP P06621
D	19	LEU	-	expression tag	UNP P06621
D	20	TYR	-	expression tag	UNP P06621
D	21	PHE	-	expression tag	UNP P06621
D	22	GLN	-	expression tag	UNP P06621
D	23	GLY	-	expression tag	UNP P06621
D	203	V44	SER	engineered mutation	UNP P06621
F	5	MET	-	initiating methionine	UNP P06621
F	6	GLY	-	expression tag	UNP P06621
F	7	SER	-	expression tag	UNP P06621
F	8	ASP	-	expression tag	UNP P06621
F	9	LYS	-	expression tag	UNP P06621
F	10	ILE	-	expression tag	UNP P06621
F	11	HIS	-	expression tag	UNP P06621
F	12	HIS	-	expression tag	UNP P06621
F	13	HIS	-	expression tag	UNP P06621
F	14	HIS	-	expression tag	UNP P06621
F	15	HIS	-	expression tag	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
F	16	HIS	-	expression tag	UNP P06621
F	17	GLU	-	expression tag	UNP P06621
F	18	ASN	-	expression tag	UNP P06621
F	19	LEU	-	expression tag	UNP P06621
F	20	TYR	-	expression tag	UNP P06621
F	21	PHE	-	expression tag	UNP P06621
F	22	GLN	-	expression tag	UNP P06621
F	23	GLY	-	expression tag	UNP P06621
F	203	V44	SER	engineered mutation	UNP P06621
H	5	MET	-	initiating methionine	UNP P06621
H	6	GLY	-	expression tag	UNP P06621
H	7	SER	-	expression tag	UNP P06621
H	8	ASP	-	expression tag	UNP P06621
H	9	LYS	-	expression tag	UNP P06621
H	10	ILE	-	expression tag	UNP P06621
H	11	HIS	-	expression tag	UNP P06621
H	12	HIS	-	expression tag	UNP P06621
H	13	HIS	-	expression tag	UNP P06621
H	14	HIS	-	expression tag	UNP P06621
H	15	HIS	-	expression tag	UNP P06621
H	16	HIS	-	expression tag	UNP P06621
H	17	GLU	-	expression tag	UNP P06621
H	18	ASN	-	expression tag	UNP P06621
H	19	LEU	-	expression tag	UNP P06621
H	20	TYR	-	expression tag	UNP P06621
H	21	PHE	-	expression tag	UNP P06621
H	22	GLN	-	expression tag	UNP P06621
H	23	GLY	-	expression tag	UNP P06621
H	203	V44	SER	engineered mutation	UNP P06621

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total Zn 7 7	0	0
3	B	5	Total Zn 5 5	0	0
3	C	5	Total Zn 5 5	0	0
3	D	9	Total Zn 9 9	0	0
3	E	8	Total Zn 8 8	0	0

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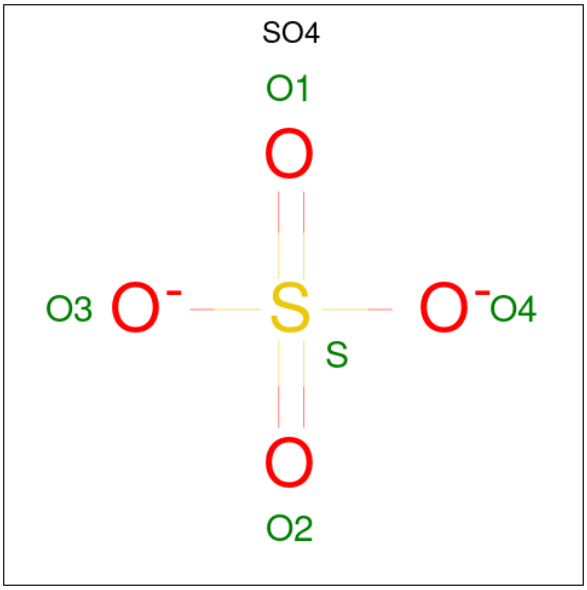
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	9	Total Zn 9 9	0	0
3	G	3	Total Zn 3 3	0	0
3	H	10	Total Zn 10 10	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	14	Total O 14 14	0	0
5	C	13	Total O 13 13	0	0
5	D	15	Total O 15 15	0	0

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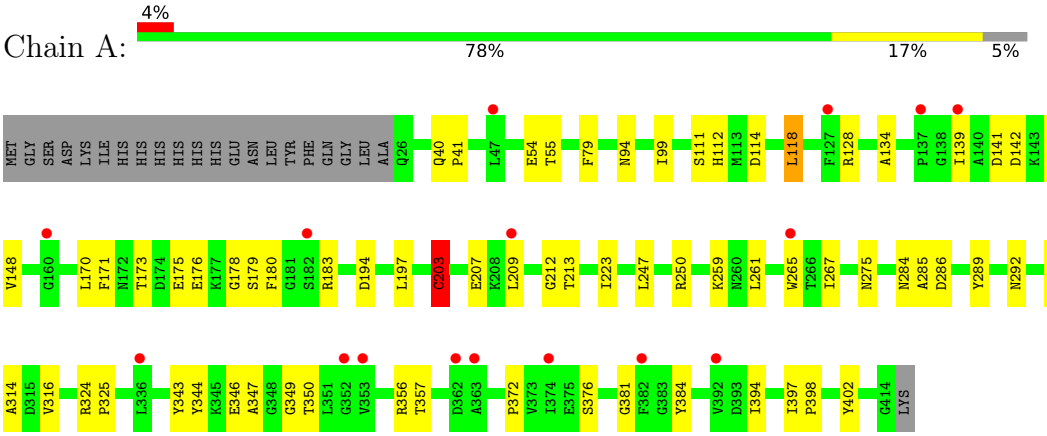
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	14	Total O 14 14	0	0
5	F	18	Total O 18 18	0	0
5	G	8	Total O 8 8	0	0
5	H	20	Total O 20 20	0	0

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.

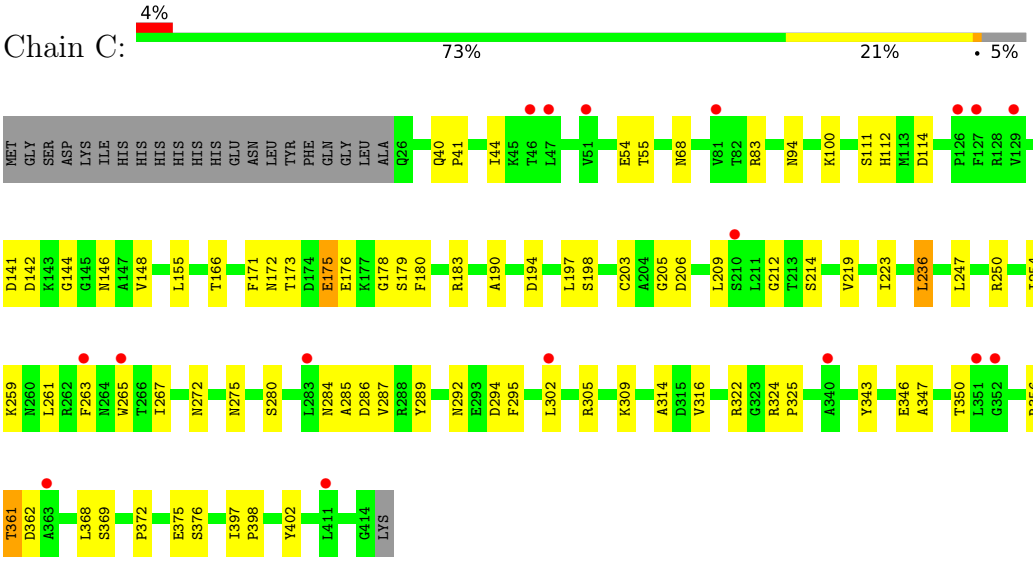
• Molecule 1: Carboxypeptidase G2

Chain A:



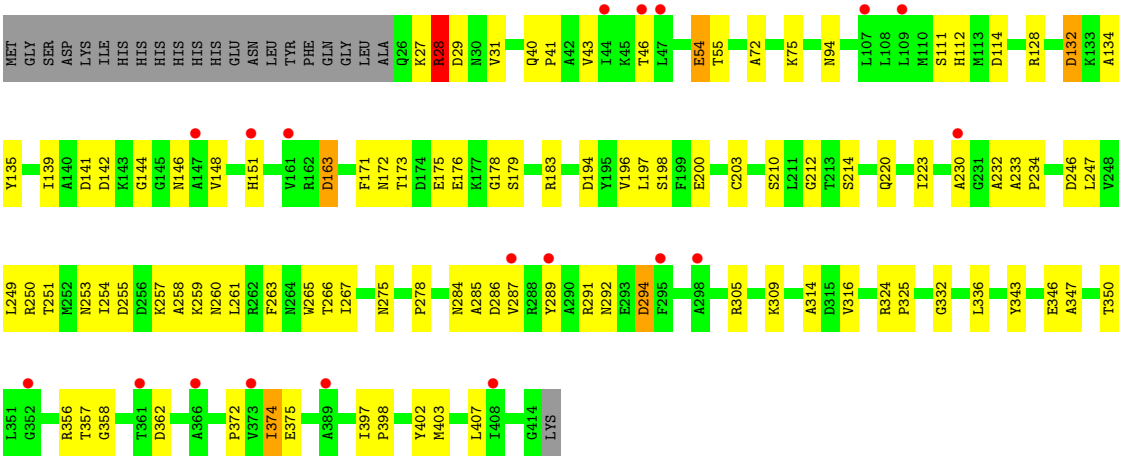
• Molecule 1: Carboxypeptidase G2

Chain C:



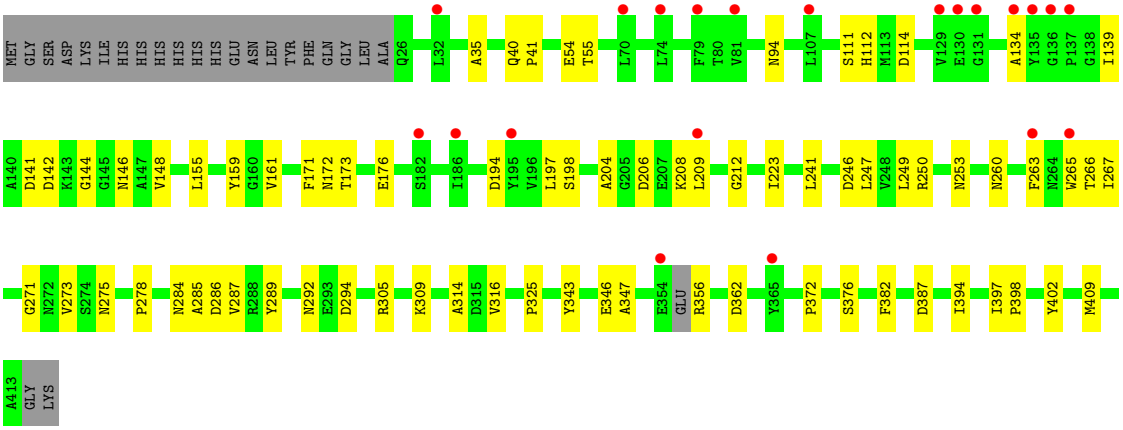
• Molecule 1: Carboxypeptidase G2

Chain E:



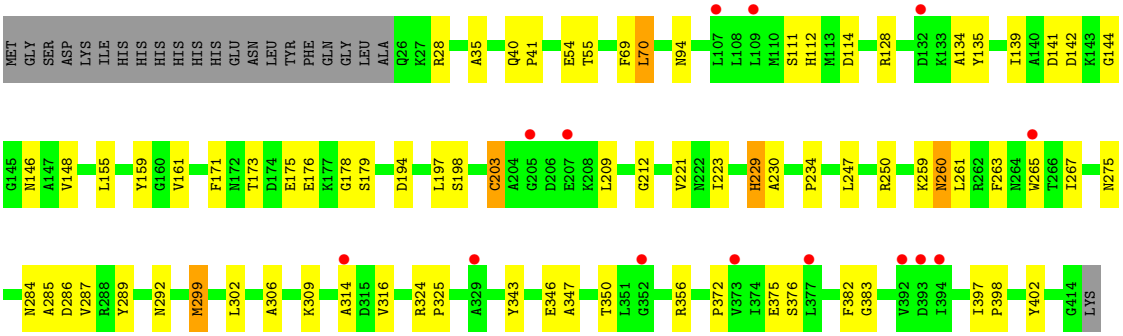
• Molecule 1: Carboxypeptidase G2

Chain G:



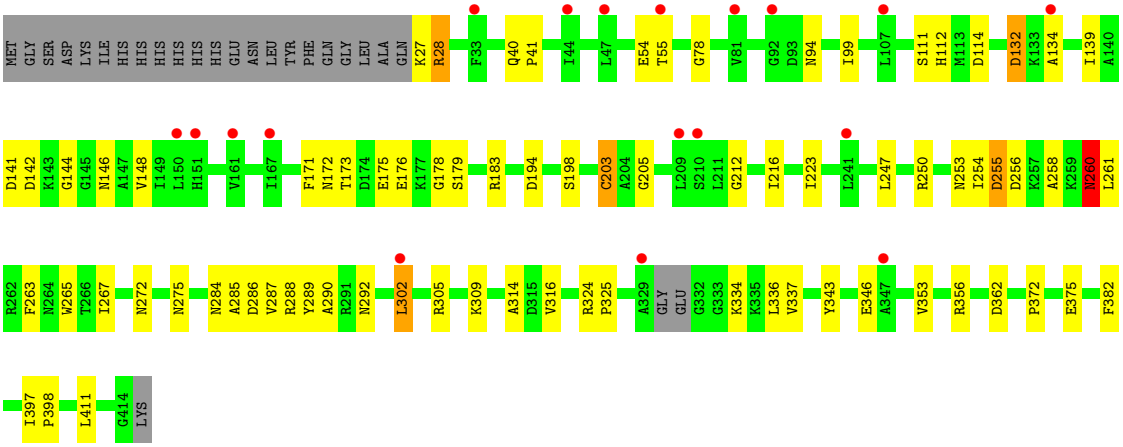
• Molecule 2: Carboxypeptidase G2

Chain B:



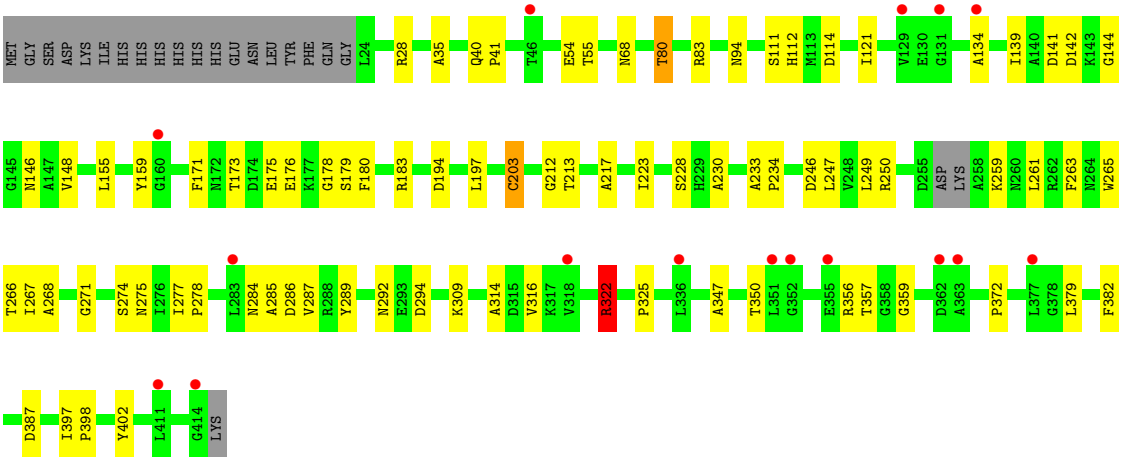
• Molecule 2: Carboxypeptidase G2

Chain D:



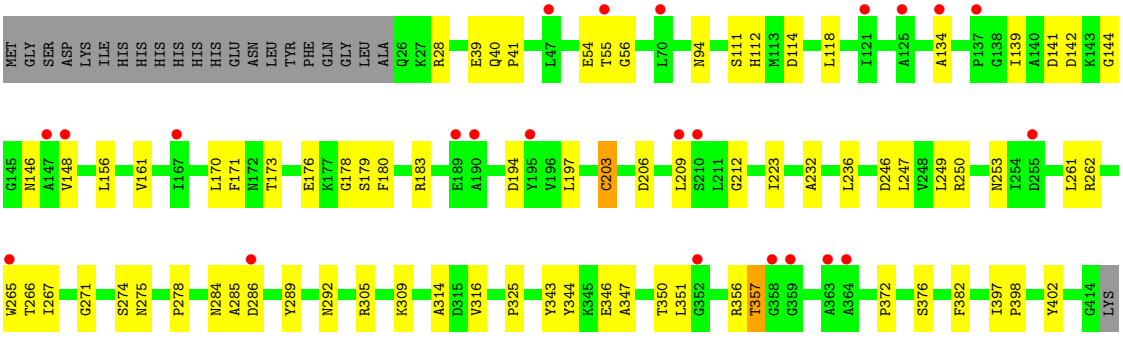
• Molecule 2: Carboxypeptidase G2

Chain F:



• Molecule 2: Carboxypeptidase G2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.12Å 188.46Å 124.50Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	41.50 – 3.11 41.50 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.50-3.11) 99.0 (41.50-3.11)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	0.39	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.271 , 0.309 0.271 , 0.305	Depositor DCC
R_{free} test set	2981 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	74.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	21541	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.25% 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: V44, SO4, ZN

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	0.67	0/2741	0.70	0/3732
1	C	0.67	0/2709	0.70	0/3697
1	E	0.68	0/2692	0.71	0/3677
1	G	0.68	0/2686	0.70	0/3667
2	B	0.68	0/2710	0.70	0/3698
2	D	0.68	0/2657	0.70	0/3628
2	F	0.68	0/2651	0.71	0/3620
2	H	0.67	0/2727	0.71	0/3714
All	All	0.68	0/21573	0.70	0/29433

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	2703	0	2529	51	0
1	C	2671	0	2484	71	0
1	E	2654	0	2407	96	0
1	G	2648	0	2422	52	0
2	B	2692	0	2435	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2642	0	2392	57	0
2	F	2635	0	2363	69	0
2	H	2710	0	2505	64	0
3	A	7	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	9	0	0	0	0
3	E	8	0	0	0	0
3	F	9	0	0	0	0
3	G	3	0	0	0	0
3	H	10	0	0	0	0
4	C	10	0	0	1	0
5	A	18	0	0	1	0
5	B	14	0	0	1	0
5	C	13	0	0	0	0
5	D	15	0	0	0	0
5	E	14	0	0	1	0
5	F	18	0	0	1	0
5	G	8	0	0	0	0
5	H	20	0	0	3	0
All	All	21541	0	19537	491	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 12.

All (491) 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:E:255:ASP:HB2	1:E:258:ALA:HB2	1.11	1.11
1:E:28:ARG:HH11	1:E:28:ARG:HB2	1.09	1.06
1:E:255:ASP:CB	1:E:258:ALA:HB2	1.86	1.05
1:C:112:HIS:CD2	1:C:175:GLU:HG2	2.01	0.96
1:E:255:ASP:HB2	1:E:258:ALA:CB	1.96	0.94
1:E:28:ARG:HH11	1:E:28:ARG:CB	1.82	0.92
2:D:255:ASP:O	2:D:255:ASP:OD1	1.92	0.87
2:D:334:LYS:O	2:D:337:VAL:HG12	1.77	0.84
1:E:28:ARG:HB2	1:E:28:ARG:NH1	1.92	0.84
2:D:216:ILE:HD12	2:D:288:ARG:HG2	1.58	0.84
2:H:28:ARG:HG2	2:H:346:GLU:O	1.79	0.82
1:C:40:GLN:O	1:C:44:ILE:CD1	2.29	0.81
2:B:247:LEU:HD13	2:B:250:ARG:NH2	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:CYS:HA	1:A:381:GLY:O	1.80	0.80
1:E:249:LEU:HD12	2:H:249:LEU:HD12	1.64	0.79
2:F:249:LEU:HD12	1:G:249:LEU:HD12	1.64	0.79
2:F:80:THR:O	2:F:80:THR:HG23	1.83	0.76
1:E:403:MET:O	1:E:407:LEU:HD23	1.87	0.75
2:D:203:V44:C3	2:D:382:PHE:CE1	2.70	0.74
2:F:80:THR:O	2:F:80:THR:CG2	2.34	0.74
1:C:40:GLN:O	1:C:44:ILE:HD13	1.89	0.73
1:G:40:GLN:HE21	1:G:394:ILE:CG2	2.01	0.72
2:B:203:V44:C2	2:B:382:PHE:HE2	2.03	0.72
1:E:200:GLU:HB2	1:E:375:GLU:OE2	1.89	0.71
1:C:259:LYS:HD2	1:C:294:ASP:OD2	1.89	0.71
1:A:40:GLN:HE21	1:A:394:ILE:CG2	2.04	0.70
1:A:175:GLU:HA	1:A:179:SER:OG	1.92	0.70
2:F:175:GLU:HA	2:F:179:SER:OG	1.91	0.70
1:C:198:SER:HB3	1:C:375:GLU:HG3	1.73	0.70
2:D:172:ASN:ND2	2:D:362:ASP:OD2	2.25	0.70
2:H:203:V44:C6	2:H:382:PHE:CD1	2.74	0.70
1:G:172:ASN:ND2	1:G:362:ASP:OD2	2.25	0.70
2:D:175:GLU:HA	2:D:179:SER:OG	1.92	0.70
2:B:175:GLU:HA	2:B:179:SER:OG	1.92	0.69
1:C:361:THR:HB	1:C:375:GLU:CD	2.12	0.69
2:D:253:ASN:OD1	2:D:305:ARG:NH1	2.26	0.69
1:E:175:GLU:HA	1:E:179:SER:OG	1.92	0.69
1:C:214:SER:H	1:C:358:GLY:HA2	1.57	0.69
2:F:259:LYS:CB	2:F:294:ASP:OD2	2.41	0.69
1:E:172:ASN:ND2	1:E:362:ASP:OD2	2.26	0.68
1:C:175:GLU:HA	1:C:179:SER:OG	1.93	0.68
2:F:259:LYS:HB2	2:F:294:ASP:OD2	1.93	0.68
1:C:44:ILE:HD12	1:C:44:ILE:H	1.59	0.68
1:C:172:ASN:ND2	1:C:362:ASP:OD2	2.25	0.68
1:E:214:SER:CB	1:E:358:GLY:HA2	2.24	0.67
2:B:128:ARG:HG3	2:B:135:TYR:HB2	1.77	0.67
2:B:247:LEU:HD13	2:B:250:ARG:HH21	1.59	0.66
1:G:40:GLN:NE2	1:G:394:ILE:HG22	2.11	0.66
1:G:253:ASN:OD1	1:G:305:ARG:NH1	2.30	0.65
2:H:356:ARG:O	2:H:357:THR:HG23	1.96	0.65
1:A:40:GLN:NE2	1:A:394:ILE:HG22	2.11	0.64
1:E:214:SER:HB2	1:E:358:GLY:HA2	1.79	0.64
2:D:203:V44:C3	2:D:382:PHE:CD1	2.81	0.64
1:G:206:ASP:O	1:G:208:LYS:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:GLU:HG2	5:H:716:HOH:O	1.98	0.63
1:E:210:SER:CB	1:E:357:THR:HG21	2.28	0.63
1:C:112:HIS:CG	1:C:175:GLU:HG2	2.33	0.63
1:E:266:THR:HA	2:H:278:PRO:HD3	1.81	0.63
1:E:253:ASN:OD1	1:E:305:ARG:NH1	2.31	0.62
2:H:261:LEU:HD12	2:H:289:TYR:HB3	1.81	0.62
2:H:203:V44:C6	2:H:382:PHE:CE1	2.82	0.62
2:F:203:V44:C7	2:F:382:PHE:CB	2.77	0.62
1:E:332:GLY:O	1:E:336:LEU:HD23	1.99	0.61
1:A:261:LEU:HD12	1:A:289:TYR:HB3	1.83	0.61
2:H:56:GLY:HA3	5:H:713:HOH:O	1.99	0.61
1:E:46:THR:CB	1:E:151:HIS:HE1	2.14	0.61
2:F:379:LEU:N	5:F:702:HOH:O	2.33	0.61
2:B:260:ASN:C	2:B:260:ASN:HD22	2.04	0.61
2:H:253:ASN:OD1	2:H:305:ARG:NH1	2.32	0.61
1:C:40:GLN:O	1:C:44:ILE:HD12	1.99	0.60
1:E:343:TYR:CD2	1:E:407:LEU:HD22	2.36	0.60
1:G:40:GLN:NE2	1:G:394:ILE:CG2	2.65	0.60
1:C:267:ILE:HB	1:C:284:ASN:HB2	1.84	0.60
1:E:267:ILE:HB	1:E:284:ASN:HB2	1.83	0.60
2:H:28:ARG:CG	2:H:346:GLU:O	2.49	0.60
2:D:111:SER:OG	2:D:146:ASN:ND2	2.35	0.60
2:D:343:TYR:O	2:D:346:GLU:HB2	2.02	0.60
1:E:198:SER:CB	1:E:375:GLU:OE1	2.50	0.60
2:B:247:LEU:HD11	2:B:306:ALA:HA	1.84	0.60
1:E:111:SER:OG	1:E:146:ASN:ND2	2.35	0.60
1:G:267:ILE:HB	1:G:284:ASN:HB2	1.83	0.60
2:B:267:ILE:HB	2:B:284:ASN:HB2	1.84	0.60
1:G:111:SER:OG	1:G:146:ASN:ND2	2.35	0.59
1:E:343:TYR:O	1:E:346:GLU:HB2	2.02	0.59
2:H:267:ILE:HB	2:H:284:ASN:HB2	1.83	0.59
2:B:111:SER:OG	2:B:146:ASN:ND2	2.35	0.59
2:B:247:LEU:CD1	2:B:306:ALA:HA	2.31	0.59
1:C:68:ASN:OD1	1:C:83:ARG:NH2	2.35	0.59
2:D:265:TRP:CE3	2:D:285:ALA:HB2	2.37	0.59
1:E:278:PRO:HD3	2:H:266:THR:HA	1.84	0.59
2:F:111:SER:OG	2:F:146:ASN:ND2	2.35	0.59
2:F:267:ILE:HB	2:F:284:ASN:HB2	1.83	0.59
2:H:265:TRP:CE3	2:H:285:ALA:HB2	2.38	0.59
1:C:111:SER:OG	1:C:146:ASN:ND2	2.35	0.59
1:E:265:TRP:CE3	1:E:285:ALA:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:TRP:CE3	1:A:285:ALA:HB2	2.38	0.59
2:F:68:ASN:OD1	2:F:83:ARG:NH2	2.36	0.59
2:B:343:TYR:O	2:B:346:GLU:HB2	2.03	0.59
1:E:46:THR:CB	1:E:151:HIS:CE1	2.86	0.59
1:A:267:ILE:HB	1:A:284:ASN:HB2	1.83	0.59
1:C:236:LEU:N	1:C:236:LEU:HD22	2.17	0.59
2:B:265:TRP:CE3	2:B:285:ALA:HB2	2.37	0.58
2:D:336:LEU:CD1	2:D:411:LEU:HD11	2.33	0.58
1:A:144:GLY:O	1:A:148:VAL:HG23	2.04	0.58
2:H:111:SER:OG	2:H:146:ASN:ND2	2.36	0.58
2:D:144:GLY:O	2:D:148:VAL:HG23	2.04	0.58
1:G:343:TYR:O	1:G:346:GLU:HB2	2.03	0.58
2:F:266:THR:HA	1:G:278:PRO:HD3	1.84	0.58
1:G:265:TRP:CE3	1:G:285:ALA:HB2	2.37	0.58
1:C:343:TYR:O	1:C:346:GLU:HB2	2.04	0.58
1:A:111:SER:OG	1:A:146:ASN:ND2	2.36	0.58
1:A:343:TYR:O	1:A:346:GLU:HB2	2.04	0.58
2:D:267:ILE:HB	2:D:284:ASN:HB2	1.85	0.58
1:C:144:GLY:O	1:C:148:VAL:HG23	2.04	0.57
1:C:176:GLU:HA	1:C:176:GLU:OE1	2.05	0.57
1:E:144:GLY:O	1:E:148:VAL:HG23	2.04	0.57
2:B:35:ALA:HB2	2:B:159:TYR:OH	2.04	0.57
1:G:260:ASN:ND2	1:G:294:ASP:OD2	2.37	0.57
2:H:343:TYR:O	2:H:346:GLU:HB2	2.04	0.57
2:B:144:GLY:O	2:B:148:VAL:HG23	2.04	0.57
1:A:176:GLU:HA	1:A:176:GLU:OE1	2.06	0.56
2:H:144:GLY:O	2:H:148:VAL:HG23	2.03	0.56
2:F:144:GLY:O	2:F:148:VAL:HG23	2.05	0.56
1:C:265:TRP:CE3	1:C:285:ALA:HB2	2.39	0.56
2:F:265:TRP:CE3	2:F:285:ALA:HB2	2.40	0.56
2:D:203:V44:C3	2:D:382:PHE:HE1	2.19	0.56
1:G:144:GLY:O	1:G:148:VAL:HG23	2.05	0.56
1:A:344:TYR:O	1:A:349:GLY:N	2.39	0.56
2:B:176:GLU:OE1	2:B:176:GLU:HA	2.06	0.56
2:D:260:ASN:ND2	2:D:290:ALA:HB3	2.21	0.56
2:F:176:GLU:HA	2:F:176:GLU:OE1	2.06	0.56
2:D:176:GLU:OE1	2:D:176:GLU:HA	2.06	0.56
2:H:203:V44:SG	2:H:203:V44:N4	2.76	0.56
1:G:176:GLU:OE1	1:G:176:GLU:HA	2.06	0.56
1:E:128:ARG:HG2	1:E:135:TYR:HB2	1.88	0.55
2:F:278:PRO:HD3	1:G:266:THR:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:GLU:HA	2:H:176:GLU:OE1	2.06	0.55
1:E:210:SER:CB	1:E:357:THR:CG2	2.85	0.55
1:A:344:TYR:C	1:A:349:GLY:HA3	2.26	0.55
1:G:35:ALA:HB2	1:G:159:TYR:OH	2.06	0.55
1:E:176:GLU:OE1	1:E:176:GLU:HA	2.07	0.55
1:A:111:SER:O	1:A:171:PHE:HA	2.07	0.55
2:B:221:VAL:HG11	2:B:247:LEU:CD2	2.37	0.55
1:C:111:SER:O	1:C:171:PHE:HA	2.07	0.55
1:C:359:GLY:O	1:C:361:THR:HG23	2.06	0.55
1:A:344:TYR:O	1:A:349:GLY:CA	2.55	0.55
2:B:155:LEU:O	2:B:159:TYR:HD1	1.90	0.55
2:D:111:SER:O	2:D:171:PHE:HA	2.08	0.54
2:F:387:ASP:HB3	2:H:232:ALA:HB2	1.88	0.54
2:B:209:LEU:HD23	2:B:376:SER:HB2	1.88	0.54
1:E:261:LEU:CD2	1:E:289:TYR:HB3	2.37	0.54
2:F:35:ALA:HB2	2:F:159:TYR:OH	2.07	0.54
2:F:261:LEU:CD2	2:F:289:TYR:HB3	2.37	0.54
1:A:40:GLN:NE2	1:A:394:ILE:CG2	2.70	0.54
1:E:28:ARG:HH11	1:E:28:ARG:CG	2.20	0.54
2:B:111:SER:O	2:B:171:PHE:HA	2.07	0.54
2:F:121:ILE:HA	2:H:236:LEU:HD11	1.90	0.54
1:C:259:LYS:CG	1:C:259:LYS:O	2.56	0.54
2:H:347:ALA:HB2	2:H:402:TYR:CD2	2.43	0.54
1:C:322:ARG:HB3	4:C:605:SO4:O2	2.08	0.54
2:F:111:SER:O	2:F:171:PHE:HA	2.07	0.54
2:H:111:SER:O	2:H:171:PHE:HA	2.07	0.54
1:G:209:LEU:HD23	1:G:376:SER:HB2	1.90	0.54
2:F:40:GLN:N	2:F:41:PRO:HD2	2.23	0.53
2:F:347:ALA:HB2	2:F:402:TYR:CD2	2.43	0.53
2:B:179:SER:OG	2:B:324:ARG:NH1	2.41	0.53
1:C:236:LEU:N	1:C:236:LEU:CD2	2.71	0.53
1:E:46:THR:HG21	1:E:151:HIS:HE1	1.74	0.53
2:F:203:V44:SG	2:F:203:V44:C4	2.96	0.53
1:A:259:LYS:HA	5:A:703:HOH:O	2.08	0.53
2:B:382:PHE:CD1	2:B:383:GLY:N	2.77	0.53
1:A:118:LEU:HD12	1:A:118:LEU:H	1.74	0.53
1:A:179:SER:OG	1:A:324:ARG:NH2	2.42	0.53
1:A:347:ALA:HB2	1:A:402:TYR:CD2	2.44	0.53
2:B:198:SER:HB3	2:B:375:GLU:CD	2.29	0.53
1:C:44:ILE:HD12	1:C:44:ILE:N	2.23	0.53
1:E:111:SER:O	1:E:171:PHE:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:SER:O	1:G:171:PHE:HA	2.08	0.53
1:C:295:PHE:CE2	1:C:322:ARG:HG3	2.44	0.53
2:D:40:GLN:N	2:D:41:PRO:HD2	2.24	0.53
1:A:397:ILE:HB	1:A:398:PRO:HD3	1.91	0.52
1:E:27:LYS:O	1:E:28:ARG:HB2	2.07	0.52
2:B:40:GLN:N	2:B:41:PRO:HD2	2.24	0.52
1:E:40:GLN:N	1:E:41:PRO:HD2	2.24	0.52
1:E:266:THR:HG21	2:H:274:SER:O	2.09	0.52
1:C:40:GLN:N	1:C:41:PRO:HD2	2.24	0.52
2:D:198:SER:HB3	2:D:375:GLU:CD	2.30	0.52
1:G:40:GLN:N	1:G:41:PRO:HD2	2.24	0.52
1:C:397:ILE:HB	1:C:398:PRO:HD3	1.91	0.52
1:C:205:GLY:HA3	2:D:205:GLY:HA3	1.91	0.52
1:E:397:ILE:HB	1:E:398:PRO:HD3	1.91	0.52
1:A:40:GLN:N	1:A:41:PRO:HD2	2.24	0.52
1:E:197:LEU:HD22	1:E:374:ILE:CG2	2.39	0.52
2:F:322:ARG:HG3	2:F:322:ARG:HH11	1.74	0.52
2:H:40:GLN:N	2:H:41:PRO:HD2	2.24	0.52
1:E:212:GLY:O	1:E:356:ARG:HA	2.10	0.51
1:C:212:GLY:O	1:C:356:ARG:HA	2.10	0.51
2:D:132:ASP:OD1	2:D:132:ASP:C	2.49	0.51
2:D:255:ASP:O	2:D:255:ASP:CG	2.48	0.51
2:B:230:ALA:HA	2:B:234:PRO:HB3	1.92	0.51
2:D:203:V44:C2	2:D:382:PHE:CE1	2.93	0.51
2:B:212:GLY:O	2:B:356:ARG:HA	2.11	0.51
1:E:214:SER:H	1:E:358:GLY:HA2	1.76	0.51
2:F:259:LYS:HB3	2:F:294:ASP:OD2	2.09	0.51
2:F:397:ILE:HB	2:F:398:PRO:HD3	1.91	0.51
1:C:209:LEU:HD23	1:C:376:SER:HB2	1.92	0.51
2:D:397:ILE:HB	2:D:398:PRO:HD3	1.92	0.51
2:F:322:ARG:HB3	2:F:322:ARG:CZ	2.40	0.51
1:G:161:VAL:HG21	1:G:409:MET:HE2	1.93	0.51
2:B:397:ILE:HB	2:B:398:PRO:HD3	1.92	0.51
1:C:112:HIS:NE2	1:C:175:GLU:HG2	2.26	0.51
1:E:179:SER:OG	1:E:324:ARG:NH2	2.44	0.51
2:H:397:ILE:HB	2:H:398:PRO:HD3	1.92	0.51
2:F:271:GLY:HA3	1:G:266:THR:O	2.12	0.50
1:G:273:VAL:HG12	1:G:275:ASN:ND2	2.26	0.50
1:E:132:ASP:C	1:E:132:ASP:OD1	2.49	0.50
1:C:112:HIS:NE2	1:C:142:ASP:HB2	2.27	0.50
1:A:212:GLY:O	1:A:356:ARG:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:SER:OG	2:D:324:ARG:NH2	2.44	0.50
1:E:46:THR:HB	1:E:151:HIS:HE1	1.77	0.50
1:C:179:SER:OG	1:C:324:ARG:NH2	2.45	0.50
2:F:212:GLY:O	2:F:356:ARG:HA	2.11	0.50
2:F:217:ALA:HB2	2:F:322:ARG:O	2.11	0.50
2:H:203:V44:SG	2:H:203:V44:C8	3.00	0.50
2:B:203:V44:C2	2:B:382:PHE:CE2	2.89	0.49
1:A:344:TYR:O	1:A:349:GLY:HA3	2.12	0.49
1:G:397:ILE:HB	1:G:398:PRO:HD3	1.92	0.49
2:B:299:MET:HA	2:B:299:MET:CE	2.43	0.49
2:D:112:HIS:NE2	2:D:142:ASP:HB2	2.28	0.49
1:E:163:ASP:OD1	1:E:163:ASP:N	2.46	0.49
2:H:344:TYR:CD2	2:H:351:LEU:HG	2.47	0.49
1:A:209:LEU:HD23	1:A:376:SER:HB2	1.95	0.49
2:F:112:HIS:NE2	2:F:142:ASP:HB2	2.28	0.49
2:B:112:HIS:NE2	2:B:142:ASP:HB2	2.28	0.49
2:H:112:HIS:NE2	2:H:142:ASP:HB2	2.28	0.49
2:H:212:GLY:O	2:H:356:ARG:HA	2.12	0.49
2:H:209:LEU:HD23	2:H:376:SER:HB2	1.94	0.48
1:C:259:LYS:O	1:C:259:LYS:CD	2.61	0.48
1:E:46:THR:HG21	1:E:151:HIS:CE1	2.48	0.48
1:E:46:THR:CG2	1:E:151:HIS:HE1	2.26	0.48
1:C:261:LEU:HD12	1:C:289:TYR:HB3	1.95	0.48
2:D:255:ASP:O	2:D:258:ALA:CB	2.61	0.48
1:E:112:HIS:NE2	1:E:142:ASP:HB2	2.28	0.48
1:G:112:HIS:NE2	1:G:142:ASP:HB2	2.27	0.48
1:A:112:HIS:NE2	1:A:142:ASP:HB2	2.28	0.48
1:E:46:THR:HG1	1:E:151:HIS:CE1	2.29	0.48
2:F:213:THR:CG2	2:F:359:GLY:HA3	2.43	0.48
1:A:178:GLY:HA3	1:A:180:PHE:CE1	2.49	0.48
1:C:180:PHE:HA	1:C:183:ARG:HD3	1.95	0.48
2:D:247:LEU:HD23	2:D:247:LEU:C	2.35	0.47
1:E:247:LEU:C	1:E:247:LEU:HD23	2.34	0.47
1:G:204:ALA:O	2:H:203:V44:C2	2.62	0.47
1:C:247:LEU:C	1:C:247:LEU:HD23	2.35	0.47
2:B:292:ASN:HD21	2:B:325:PRO:HB2	1.80	0.47
1:E:29:ASP:O	1:E:31:VAL:N	2.44	0.47
1:A:94:ASN:OD1	1:A:173:THR:HG22	2.15	0.47
1:A:250:ARG:O	1:A:305:ARG:HD3	2.15	0.47
2:B:221:VAL:HG11	2:B:247:LEU:HD21	1.94	0.47
1:C:272:ASN:OD1	2:D:272:ASN:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:LEU:CD2	2:D:289:TYR:HB3	2.44	0.47
1:C:292:ASN:HD21	1:C:325:PRO:HB2	1.80	0.47
2:H:250:ARG:O	2:H:305:ARG:HD3	2.15	0.47
1:E:347:ALA:HB2	1:E:402:TYR:CD1	2.50	0.47
1:G:212:GLY:O	1:G:356:ARG:CB	2.63	0.47
1:G:247:LEU:C	1:G:247:LEU:HD23	2.35	0.47
2:B:347:ALA:HB2	2:B:402:TYR:CD1	2.50	0.47
1:G:292:ASN:HD21	1:G:325:PRO:HB2	1.80	0.47
1:A:247:LEU:HD23	1:A:247:LEU:C	2.35	0.46
1:C:259:LYS:O	1:C:259:LYS:HD3	2.16	0.46
1:C:259:LYS:O	1:C:259:LYS:HG3	2.15	0.46
2:B:247:LEU:HA	2:B:250:ARG:HG2	1.98	0.46
1:C:250:ARG:O	1:C:305:ARG:HD3	2.16	0.46
1:A:183:ARG:HH11	1:A:183:ARG:HG2	1.81	0.46
2:B:299:MET:CE	2:B:302:LEU:CD2	2.93	0.46
1:E:46:THR:HB	1:E:151:HIS:CE1	2.50	0.46
1:G:347:ALA:HB2	1:G:402:TYR:CD1	2.51	0.46
2:H:94:ASN:OD1	2:H:173:THR:HG22	2.16	0.46
2:D:212:GLY:O	2:D:356:ARG:HA	2.15	0.46
1:E:291:ARG:O	1:E:294:ASP:OD1	2.34	0.46
2:B:203:V44:C3	2:B:382:PHE:CE2	2.99	0.46
2:B:299:MET:HE2	2:B:302:LEU:HD23	1.98	0.46
2:H:203:V44:C6	2:H:382:PHE:HD1	2.28	0.46
1:A:247:LEU:HA	1:A:250:ARG:HG2	1.97	0.46
2:H:309:LYS:HD3	2:H:314:ALA:O	2.17	0.46
1:A:141:ASP:HA	1:A:142:ASP:HA	1.69	0.45
2:F:247:LEU:HD23	2:F:247:LEU:C	2.35	0.45
1:C:197:LEU:HD12	1:C:197:LEU:N	2.31	0.45
2:D:254:ILE:HD12	2:D:302:LEU:HD23	1.97	0.45
2:H:247:LEU:HA	2:H:250:ARG:HG2	1.99	0.45
1:C:219:VAL:HG11	1:C:302:LEU:HD21	1.98	0.45
2:D:139:ILE:O	2:D:144:GLY:N	2.50	0.45
2:F:121:ILE:HA	2:H:236:LEU:CD1	2.46	0.45
2:H:197:LEU:HD12	2:H:197:LEU:N	2.31	0.45
1:A:223:ILE:HG12	1:A:316:VAL:HG22	1.99	0.45
1:C:44:ILE:CD1	1:C:44:ILE:H	2.26	0.45
1:C:347:ALA:HB2	1:C:402:TYR:CD1	2.50	0.45
2:F:292:ASN:HD21	2:F:325:PRO:HB2	1.81	0.45
2:F:387:ASP:CB	2:H:232:ALA:HB2	2.46	0.45
1:G:247:LEU:HA	1:G:250:ARG:HG2	1.99	0.45
1:G:250:ARG:O	1:G:305:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:HA	1:C:250:ARG:HG2	1.99	0.45
1:E:232:ALA:HB2	1:G:387:ASP:HB3	1.98	0.45
1:E:259:LYS:CB	1:E:294:ASP:OD2	2.64	0.45
2:F:322:ARG:HH11	2:F:322:ARG:CG	2.29	0.45
1:C:361:THR:CB	1:C:375:GLU:CD	2.83	0.45
1:E:247:LEU:HA	1:E:250:ARG:HG2	1.98	0.45
1:A:79:PHE:CE1	1:A:99:ILE:HG22	2.52	0.45
2:F:223:ILE:HG12	2:F:316:VAL:HG22	1.98	0.45
1:C:141:ASP:HA	1:C:142:ASP:HA	1.68	0.44
1:E:249:LEU:CD1	2:H:249:LEU:HD12	2.42	0.44
1:G:223:ILE:HG12	1:G:316:VAL:HG22	1.98	0.44
2:D:292:ASN:HD21	2:D:325:PRO:HB2	1.82	0.44
1:E:249:LEU:HD12	2:H:249:LEU:CD1	2.43	0.44
1:C:139:ILE:O	1:C:144:GLY:N	2.51	0.44
1:E:250:ARG:O	1:E:305:ARG:HD3	2.17	0.44
1:G:155:LEU:O	1:G:159:TYR:HD2	2.00	0.44
2:H:292:ASN:HD21	2:H:325:PRO:HB2	1.83	0.44
2:B:139:ILE:O	2:B:144:GLY:N	2.50	0.44
2:B:223:ILE:HG12	2:B:316:VAL:HG22	1.98	0.44
2:D:134:ALA:O	2:D:139:ILE:HD13	2.18	0.44
1:E:223:ILE:HG12	1:E:316:VAL:HG22	1.99	0.44
2:H:180:PHE:HA	2:H:183:ARG:HD3	1.98	0.44
1:E:28:ARG:NH1	1:E:28:ARG:CG	2.79	0.44
1:E:257:LYS:HA	1:E:260:ASN:HA	1.99	0.44
2:F:141:ASP:HA	2:F:142:ASP:HA	1.69	0.44
2:F:155:LEU:O	2:F:159:TYR:HD2	2.01	0.44
2:F:249:LEU:HD11	1:G:246:ASP:HA	1.99	0.44
2:B:55:THR:O	2:B:114:ASP:HA	2.18	0.44
1:C:254:ILE:O	1:C:255:ASP:C	2.55	0.44
1:E:139:ILE:O	1:E:144:GLY:N	2.50	0.44
2:F:180:PHE:HA	2:F:183:ARG:HD3	2.00	0.44
1:C:309:LYS:HD3	1:C:314:ALA:O	2.18	0.44
2:D:261:LEU:C	2:D:261:LEU:HD13	2.38	0.44
1:E:54:GLU:CB	5:E:706:HOH:O	2.65	0.44
1:G:197:LEU:HD12	1:G:197:LEU:N	2.33	0.44
2:H:223:ILE:HG12	2:H:316:VAL:HG22	2.00	0.44
2:B:197:LEU:HD12	2:B:197:LEU:N	2.32	0.44
1:G:134:ALA:O	1:G:139:ILE:HD13	2.18	0.44
2:H:134:ALA:O	2:H:139:ILE:HD13	2.18	0.44
1:A:292:ASN:HD21	1:A:325:PRO:HB2	1.83	0.44
2:D:55:THR:O	2:D:114:ASP:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ALA:HA	1:E:234:PRO:HG3	2.00	0.44
1:E:234:PRO:HD3	2:H:262:ARG:HH12	1.83	0.44
1:E:309:LYS:HD3	1:E:314:ALA:O	2.17	0.44
1:E:343:TYR:HD2	1:E:407:LEU:CD2	2.30	0.44
2:F:261:LEU:C	2:F:261:LEU:HD13	2.39	0.44
1:A:55:THR:O	1:A:114:ASP:HA	2.18	0.43
1:A:139:ILE:O	1:A:144:GLY:N	2.51	0.43
2:B:382:PHE:CD1	2:B:382:PHE:C	2.92	0.43
2:D:263:PHE:CD2	2:D:287:VAL:HG22	2.53	0.43
1:E:249:LEU:HD11	2:H:246:ASP:HA	2.00	0.43
2:F:134:ALA:O	2:F:139:ILE:HD13	2.17	0.43
1:G:139:ILE:O	1:G:144:GLY:N	2.51	0.43
1:A:197:LEU:N	1:A:197:LEU:HD12	2.33	0.43
2:D:309:LYS:HD3	2:D:314:ALA:O	2.18	0.43
2:F:55:THR:O	2:F:114:ASP:HA	2.18	0.43
2:F:197:LEU:N	2:F:197:LEU:HD12	2.33	0.43
2:F:230:ALA:HA	2:F:234:PRO:HG3	2.01	0.43
2:F:247:LEU:HA	2:F:250:ARG:HG2	1.99	0.43
2:B:134:ALA:O	2:B:139:ILE:HD13	2.18	0.43
1:C:55:THR:O	1:C:114:ASP:HA	2.19	0.43
2:F:183:ARG:HH12	2:F:322:ARG:HG3	1.83	0.43
2:B:142:ASP:N	5:B:701:HOH:O	2.30	0.43
1:E:134:ALA:O	1:E:139:ILE:HD13	2.17	0.43
1:E:251:THR:O	1:E:254:ILE:HG13	2.19	0.43
2:F:139:ILE:O	2:F:144:GLY:N	2.51	0.43
2:F:233:ALA:N	2:F:234:PRO:HD3	2.33	0.43
1:G:194:ASP:O	1:G:372:PRO:HD2	2.19	0.43
1:G:309:LYS:HD3	1:G:314:ALA:O	2.19	0.43
2:D:223:ILE:HG12	2:D:316:VAL:HG22	2.00	0.43
1:E:55:THR:O	1:E:114:ASP:HA	2.18	0.43
1:E:72:ALA:O	1:E:75:LYS:HG2	2.18	0.43
1:A:194:ASP:O	1:A:372:PRO:HD2	2.19	0.43
2:B:229:HIS:O	2:B:230:ALA:HB3	2.18	0.43
2:B:299:MET:CE	2:B:302:LEU:HD23	2.48	0.43
1:C:194:ASP:O	1:C:372:PRO:HD2	2.18	0.43
2:H:139:ILE:O	2:H:144:GLY:N	2.51	0.43
1:C:134:ALA:O	1:C:139:ILE:HD13	2.18	0.43
1:C:223:ILE:HG12	1:C:316:VAL:HG22	1.99	0.43
1:E:343:TYR:HD2	1:E:407:LEU:HD22	1.81	0.43
2:F:194:ASP:O	2:F:372:PRO:HD2	2.19	0.43
2:F:228:SER:OG	2:F:277:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:ASP:O	2:H:372:PRO:HD2	2.19	0.43
1:E:46:THR:OG1	1:E:151:HIS:CE1	2.72	0.43
2:F:114:ASP:HB3	2:F:173:THR:O	2.19	0.43
2:F:274:SER:O	1:G:266:THR:HG21	2.19	0.43
2:F:309:LYS:HD3	2:F:314:ALA:O	2.18	0.43
2:B:309:LYS:HD3	2:B:314:ALA:O	2.19	0.43
1:C:94:ASN:OD1	1:C:173:THR:HG23	2.19	0.43
1:E:233:ALA:N	1:E:234:PRO:HD3	2.34	0.43
2:H:350:THR:HG23	2:H:350:THR:O	2.19	0.43
2:B:69:PHE:HD2	2:B:70:LEU:HD13	1.83	0.43
2:B:114:ASP:HB3	2:B:173:THR:O	2.19	0.43
1:C:325:PRO:HG3	1:C:368:LEU:HD11	2.00	0.43
1:E:263:PHE:CD2	1:E:287:VAL:HG22	2.54	0.43
1:A:170:LEU:HD23	1:A:171:PHE:N	2.34	0.42
2:B:194:ASP:O	2:B:372:PRO:HD2	2.19	0.42
1:C:263:PHE:CD2	1:C:287:VAL:HG22	2.54	0.42
2:D:247:LEU:HA	2:D:250:ARG:HG2	2.00	0.42
1:E:261:LEU:HD13	1:E:261:LEU:C	2.39	0.42
1:G:94:ASN:OD1	1:G:173:THR:HG23	2.19	0.42
2:D:78:GLY:C	2:D:99:ILE:HD12	2.40	0.42
2:D:114:ASP:HB3	2:D:173:THR:O	2.19	0.42
2:D:178:GLY:O	2:D:179:SER:HB2	2.19	0.42
2:H:114:ASP:HB3	2:H:173:THR:O	2.19	0.42
2:B:94:ASN:OD1	2:B:173:THR:HG23	2.19	0.42
2:B:198:SER:HB3	2:B:375:GLU:OE2	2.19	0.42
1:C:114:ASP:HB3	1:C:173:THR:O	2.19	0.42
1:C:190:ALA:HB3	1:C:369:SER:OG	2.19	0.42
1:E:292:ASN:HD21	1:E:325:PRO:HB2	1.83	0.42
2:F:213:THR:HA	2:F:357:THR:O	2.19	0.42
1:G:382:PHE:CE1	2:H:203:V44:C9	3.02	0.42
1:G:397:ILE:N	1:G:398:PRO:CD	2.83	0.42
2:H:55:THR:O	2:H:114:ASP:HA	2.19	0.42
1:E:253:ASN:OD1	1:E:253:ASN:C	2.58	0.42
1:A:309:LYS:HD3	1:A:314:ALA:O	2.19	0.42
2:B:397:ILE:N	2:B:398:PRO:CD	2.83	0.42
1:C:178:GLY:O	1:C:179:SER:HB2	2.19	0.42
2:D:255:ASP:O	2:D:258:ALA:HB3	2.19	0.42
2:F:246:ASP:HA	1:G:249:LEU:HD11	2.01	0.42
1:G:55:THR:O	1:G:114:ASP:HA	2.19	0.42
1:A:114:ASP:HB3	1:A:173:THR:O	2.20	0.42
1:A:213:THR:HA	1:A:357:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:LEU:O	2:B:159:TYR:CD1	2.72	0.42
2:D:94:ASN:OD1	2:D:173:THR:HG23	2.20	0.42
1:E:196:VAL:C	1:E:197:LEU:HD23	2.40	0.42
2:F:94:ASN:OD1	2:F:173:THR:HG23	2.20	0.42
1:E:246:ASP:HA	2:H:249:LEU:HD11	2.01	0.42
2:F:397:ILE:N	2:F:398:PRO:CD	2.83	0.42
1:G:141:ASP:HA	1:G:142:ASP:HA	1.70	0.42
1:A:134:ALA:O	1:A:139:ILE:HD13	2.18	0.42
2:B:350:THR:HG23	2:B:350:THR:O	2.20	0.42
2:D:194:ASP:O	2:D:372:PRO:HD2	2.20	0.42
1:E:266:THR:O	2:H:271:GLY:HA3	2.19	0.42
1:E:350:THR:HG23	1:E:350:THR:O	2.20	0.42
2:D:27:LYS:O	2:D:28:ARG:HB2	2.20	0.42
1:E:94:ASN:OD1	1:E:173:THR:HG23	2.20	0.42
1:E:397:ILE:N	1:E:398:PRO:CD	2.83	0.42
1:E:403:MET:O	1:E:407:LEU:CD2	2.64	0.42
2:F:350:THR:O	2:F:350:THR:HG23	2.20	0.42
1:G:263:PHE:CD2	1:G:287:VAL:HG22	2.55	0.42
2:H:118:LEU:HD12	5:H:717:HOH:O	2.20	0.42
2:B:141:ASP:HA	2:B:142:ASP:HA	1.70	0.41
2:H:141:ASP:HA	2:H:142:ASP:HA	1.69	0.41
2:B:178:GLY:O	2:B:179:SER:HB2	2.20	0.41
2:B:260:ASN:HD22	2:B:261:LEU:N	2.18	0.41
2:B:263:PHE:CD2	2:B:287:VAL:HG22	2.55	0.41
2:H:178:GLY:O	2:H:179:SER:HB3	2.20	0.41
2:H:397:ILE:N	2:H:398:PRO:CD	2.83	0.41
2:D:289:TYR:CD1	2:D:289:TYR:N	2.89	0.41
1:C:214:SER:N	1:C:358:GLY:HA2	2.28	0.41
1:A:203:CYS:HB2	1:A:384:TYR:OH	2.21	0.41
2:D:260:ASN:ND2	2:D:260:ASN:C	2.74	0.41
1:E:178:GLY:O	1:E:179:SER:HB2	2.21	0.41
2:F:28:ARG:HE	2:F:28:ARG:HB3	1.70	0.41
1:A:178:GLY:O	1:A:179:SER:HB2	2.20	0.41
1:A:350:THR:HG22	1:A:350:THR:O	2.21	0.41
1:C:100:LYS:HD3	1:C:166:THR:OG1	2.21	0.41
2:D:250:ARG:O	2:D:305:ARG:HD3	2.21	0.41
2:D:397:ILE:N	2:D:398:PRO:CD	2.83	0.41
1:E:114:ASP:HB3	1:E:173:THR:O	2.20	0.41
1:A:289:TYR:CD1	1:A:289:TYR:N	2.88	0.41
2:B:289:TYR:CD1	2:B:289:TYR:N	2.89	0.41
1:C:350:THR:HG23	1:C:350:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ILE:N	1:C:398:PRO:CD	2.83	0.41
2:D:203:V44:SG	2:D:203:V44:C4	3.08	0.41
2:H:170:LEU:HD23	2:H:171:PHE:N	2.36	0.41
1:E:43:VAL:HG22	1:E:151:HIS:CG	2.56	0.41
1:E:141:ASP:HA	1:E:142:ASP:HA	1.69	0.41
1:E:194:ASP:O	1:E:372:PRO:HD2	2.21	0.41
2:F:266:THR:O	1:G:271:GLY:HA3	2.21	0.41
2:F:322:ARG:CG	2:F:322:ARG:NH1	2.84	0.41
2:H:156:LEU:HD22	2:H:161:VAL:HG21	2.03	0.41
2:H:289:TYR:CD1	2:H:289:TYR:N	2.89	0.41
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.96	0.41
1:C:289:TYR:CD1	1:C:289:TYR:N	2.89	0.41
2:D:141:ASP:HA	2:D:142:ASP:HA	1.69	0.41
2:H:356:ARG:CZ	2:H:356:ARG:HB2	2.51	0.40
1:C:236:LEU:CD2	1:C:236:LEU:H	2.34	0.40
1:E:46:THR:OG1	1:E:151:HIS:NE2	2.48	0.40
1:E:294:ASP:OD1	1:E:294:ASP:N	2.43	0.40
1:G:289:TYR:CD1	1:G:289:TYR:N	2.89	0.40
1:A:180:PHE:HA	1:A:183:ARG:HD3	2.03	0.40
1:A:397:ILE:N	1:A:398:PRO:CD	2.84	0.40
2:F:263:PHE:CD2	2:F:287:VAL:HG22	2.57	0.40
2:F:268:ALA:HB3	1:G:241:LEU:HD13	2.04	0.40
2:D:198:SER:HB3	2:D:375:GLU:OE2	2.21	0.40
1:E:220:GLN:HE21	1:E:220:GLN:HB2	1.71	0.40
2:F:289:TYR:CD1	2:F:289:TYR:N	2.89	0.40
2:D:253:ASN:O	2:D:256:ASP:CB	2.70	0.40
2:F:178:GLY:O	2:F:179:SER:HB2	2.21	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	387/411 (94%)	354 (92%)	30 (8%)	3 (1%)	19	53
1	C	387/411 (94%)	346 (89%)	34 (9%)	7 (2%)	8	33
1	E	387/411 (94%)	352 (91%)	33 (8%)	2 (0%)	29	63
1	G	383/411 (93%)	353 (92%)	29 (8%)	1 (0%)	41	73
2	B	386/411 (94%)	348 (90%)	35 (9%)	3 (1%)	19	53
2	D	381/411 (93%)	347 (91%)	31 (8%)	3 (1%)	19	53
2	F	384/411 (93%)	349 (91%)	33 (9%)	2 (0%)	29	63
2	H	386/411 (94%)	355 (92%)	29 (8%)	2 (0%)	29	63
All	All	3081/3288 (94%)	2804 (91%)	254 (8%)	23 (1%)	22	56

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	206	ASP
1	C	255	ASP
1	C	257	LYS
1	E	28	ARG
2	F	322	ARG
2	B	259	LYS
1	C	361	THR
2	D	260	ASN
1	A	203	CYS
1	A	207	GLU
2	B	54	GLU
2	B	161	VAL
1	C	54	GLU
2	D	54	GLU
1	E	54	GLU
2	F	54	GLU
1	G	54	GLU
1	A	54	GLU
2	D	28	ARG
2	H	54	GLU
1	C	359	GLY
2	H	206	ASP
1	C	360	GLY

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	239/315 (76%)	234 (98%)	5 (2%)	53 78
1	C	231/315 (73%)	225 (97%)	6 (3%)	46 74
1	E	227/315 (72%)	218 (96%)	9 (4%)	31 64
1	G	228/315 (72%)	226 (99%)	2 (1%)	78 91
2	B	229/314 (73%)	222 (97%)	7 (3%)	40 69
2	D	225/314 (72%)	217 (96%)	8 (4%)	35 66
2	F	215/314 (68%)	211 (98%)	4 (2%)	57 80
2	H	236/314 (75%)	233 (99%)	3 (1%)	69 86
All	All	1830/2516 (73%)	1786 (98%)	44 (2%)	49 75

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	128	ARG
1	A	203	CYS
1	A	275	ASN
1	A	286	ASP
2	B	28	ARG
2	B	70	LEU
2	B	229	HIS
2	B	260	ASN
2	B	275	ASN
2	B	286	ASP
2	B	299	MET
1	C	175	GLU
1	C	203	CYS
1	C	236	LEU
1	C	275	ASN
1	C	280	SER
1	C	286	ASP
2	D	132	ASP

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Mol	Chain	Res	Type
2	D	183	ARG
2	D	255	ASP
2	D	260	ASN
2	D	275	ASN
2	D	286	ASP
2	D	302	LEU
2	D	353	VAL
1	E	28	ARG
1	E	132	ASP
1	E	163	ASP
1	E	183	ARG
1	E	203	CYS
1	E	275	ASN
1	E	286	ASP
1	E	294	ASP
1	E	374	ILE
2	F	80	THR
2	F	275	ASN
2	F	286	ASP
2	F	322	ARG
1	G	198	SER
1	G	286	ASP
2	H	275	ASN
2	H	286	ASP
2	H	357	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	68	ASN
1	A	146	ASN
1	A	220	GLN
1	A	275	ASN
1	A	284	ASN
2	B	146	ASN
2	B	220	GLN
2	B	260	ASN
2	B	275	ASN
2	B	284	ASN
2	B	307	GLN
1	C	146	ASN

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Mol	Chain	Res	Type
1	C	220	GLN
1	C	272	ASN
1	C	275	ASN
1	C	284	ASN
1	C	307	GLN
2	D	146	ASN
2	D	220	GLN
2	D	275	ASN
2	D	284	ASN
2	D	307	GLN
1	E	146	ASN
1	E	220	GLN
1	E	272	ASN
1	E	275	ASN
1	E	284	ASN
1	E	307	GLN
2	F	40	GLN
2	F	146	ASN
2	F	220	GLN
2	F	275	ASN
2	F	284	ASN
2	F	307	GLN
1	G	40	GLN
1	G	146	ASN
1	G	220	GLN
1	G	275	ASN
1	G	284	ASN
1	G	307	GLN
2	H	26	GLN
2	H	146	ASN
2	H	220	GLN
2	H	275	ASN
2	H	284	ASN
2	H	307	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
2	V44	H	203	3,2	17,21,22	1.33	2 (11%)	12,28,30	1.93	3 (25%)
2	V44	B	203	3,2	17,21,22	1.37	2 (11%)	12,28,30	1.21	2 (16%)
2	V44	F	203	3,2	17,21,22	1.15	2 (11%)	12,28,30	1.50	3 (25%)
2	V44	D	203	3,2	17,21,22	1.35	2 (11%)	12,28,30	1.43	3 (25%)

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	V44	H	203	3,2	-	3/6/16/18	0/2/2/2
2	V44	B	203	3,2	-	4/6/16/18	0/2/2/2
2	V44	F	203	3,2	-	4/6/16/18	0/2/2/2
2	V44	D	203	3,2	-	4/6/16/18	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	203	V44	C5-N3	3.49	1.40	1.34
2	B	203	V44	C1-N1	3.33	1.39	1.34
2	D	203	V44	C1-N1	3.15	1.39	1.34
2	B	203	V44	C5-N3	3.14	1.39	1.34
2	H	203	V44	C5-N3	3.07	1.39	1.34
2	H	203	V44	C1-N1	3.06	1.39	1.34
2	F	203	V44	C1-N1	2.58	1.38	1.34
2	F	203	V44	C5-N3	2.56	1.38	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	203	V44	CB-SG-C10	-4.75	94.06	102.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	203	V44	CB-SG-C10	-2.85	97.29	102.13
2	F	203	V44	CB-SG-C10	-2.82	97.35	102.13
2	H	203	V44	C9-C1-N1	2.59	130.02	125.08
2	F	203	V44	C9-C5-N3	2.55	129.94	125.08
2	H	203	V44	C9-C5-N3	2.48	129.81	125.08
2	D	203	V44	C9-C1-N1	2.32	129.50	125.08
2	B	203	V44	C9-C5-N3	2.26	129.38	125.08
2	D	203	V44	C9-C5-N3	2.20	129.28	125.08
2	B	203	V44	C9-C1-N1	2.07	129.03	125.08
2	F	203	V44	C9-C1-N1	2.04	128.97	125.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	203	V44	SG-C10-C9-C1
2	B	203	V44	SG-C10-C9-C5
2	B	203	V44	C-CA-CB-SG
2	B	203	V44	N-CA-CB-SG
2	D	203	V44	SG-C10-C9-C1
2	D	203	V44	SG-C10-C9-C5
2	D	203	V44	C-CA-CB-SG
2	D	203	V44	N-CA-CB-SG
2	F	203	V44	SG-C10-C9-C1
2	F	203	V44	SG-C10-C9-C5
2	F	203	V44	C-CA-CB-SG
2	F	203	V44	N-CA-CB-SG
2	H	203	V44	SG-C10-C9-C1
2	H	203	V44	SG-C10-C9-C5
2	H	203	V44	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	203	V44	7	0
2	B	203	V44	3	0
2	F	203	V44	2	0
2	D	203	V44	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 58 ligands modelled in this entry, 56 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	SO4	C	604	-	4,4,4	0.34	0	6,6,6	0.05	0
4	SO4	C	605	-	4,4,4	0.37	0	6,6,6	0.05	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
4	C	605	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	389/411 (94%)	0.29	16 (4%)	37	18	55, 68, 80, 90	0
1	C	389/411 (94%)	0.36	18 (4%)	32	15	56, 70, 87, 102	0
1	E	389/411 (94%)	0.31	19 (4%)	29	13	55, 77, 92, 99	0
1	G	387/411 (94%)	0.34	21 (5%)	25	12	54, 74, 88, 99	0
2	B	388/411 (94%)	0.29	14 (3%)	42	22	55, 73, 86, 97	0
2	D	385/411 (93%)	0.35	18 (4%)	31	14	54, 76, 94, 102	0
2	F	388/411 (94%)	0.25	16 (4%)	37	18	51, 69, 83, 88	0
2	H	388/411 (94%)	0.38	23 (5%)	22	10	54, 69, 83, 94	0
All	All	3103/3288 (94%)	0.32	145 (4%)	31	14	51, 72, 88, 102	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	359	GLY	4.8
2	F	160	GLY	4.2
2	D	347	ALA	4.2
1	A	352	GLY	4.0
1	C	46	THR	3.9
1	A	362	ASP	3.9
1	C	47	LEU	3.8
1	C	129	VAL	3.8
2	B	314	ALA	3.8
1	G	134	ALA	3.8
2	B	205	GLY	3.6
2	D	209	LEU	3.6
2	H	147	ALA	3.5
1	A	137	PRO	3.5
2	B	392	VAL	3.5
1	C	134	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	210	SER	3.5
2	F	377	LEU	3.3
1	A	209	LEU	3.2
2	H	286	ASP	3.2
1	C	265	TRP	3.2
1	C	51	VAL	3.2
2	D	241	LEU	3.2
1	G	70	LEU	3.2
1	G	209	LEU	3.2
2	F	352	GLY	3.1
2	H	352	GLY	3.1
2	F	129	VAL	3.1
1	G	195	TYR	3.1
2	B	393	ASP	3.1
2	B	352	GLY	3.0
1	E	408	ILE	2.9
1	G	130	GLU	2.9
2	H	137	PRO	2.9
1	E	46	THR	2.9
1	E	47	LEU	2.9
2	H	121	ILE	2.9
1	G	265	TRP	2.9
2	D	329	ALA	2.9
1	C	351	LEU	2.8
1	A	363	ALA	2.8
1	G	135	TYR	2.8
2	F	414	GLY	2.8
2	H	125	ALA	2.8
1	G	186	ILE	2.8
2	F	131	GLY	2.8
1	C	126	PRO	2.7
2	H	265	TRP	2.7
2	H	210	SER	2.6
1	A	139	ILE	2.6
2	H	47	LEU	2.6
1	C	352	GLY	2.6
1	E	151	HIS	2.6
2	B	132	ASP	2.6
2	B	207	GLU	2.5
2	H	189	GLU	2.5
2	F	355	GLU	2.5
2	F	46	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	209	LEU	2.5
2	H	358	GLY	2.5
2	B	265	TRP	2.5
1	A	392	VAL	2.5
1	E	366	ALA	2.5
2	H	255	ASP	2.5
1	G	182	SER	2.5
2	H	55	THR	2.5
1	C	263	PHE	2.5
1	E	361	THR	2.5
1	E	389	ALA	2.5
1	G	365	TYR	2.5
1	C	127	PHE	2.4
1	C	411	LEU	2.4
1	E	107	LEU	2.4
2	H	190	ALA	2.4
2	F	134	ALA	2.4
2	D	44	ILE	2.4
1	A	47	LEU	2.4
2	D	92	GLY	2.4
2	D	161	VAL	2.4
2	F	336	LEU	2.4
2	D	81	VAL	2.4
2	D	151	HIS	2.4
1	E	161	VAL	2.4
1	E	295	PHE	2.4
1	A	265	TRP	2.4
1	E	44	ILE	2.4
1	G	107	LEU	2.4
1	G	81	VAL	2.3
1	G	129	VAL	2.3
1	E	147	ALA	2.3
1	A	353	VAL	2.3
1	E	373	VAL	2.3
2	F	362	ASP	2.3
1	A	374	ILE	2.3
1	G	32	LEU	2.3
1	A	160	GLY	2.3
2	D	107	LEU	2.3
1	G	79	PHE	2.3
2	F	351	LEU	2.3
1	G	263	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	137	PRO	2.3
1	G	354	GLU	2.3
2	B	377	LEU	2.3
2	D	150	LEU	2.3
2	F	283	LEU	2.3
2	H	70	LEU	2.3
1	A	382	PHE	2.3
1	C	340	ALA	2.3
1	E	298	ALA	2.3
1	G	131	GLY	2.2
1	G	136	GLY	2.2
2	B	394	ILE	2.2
2	F	318	VAL	2.2
1	A	336	LEU	2.2
2	D	33	PHE	2.2
1	G	74	LEU	2.2
2	H	364	ALA	2.2
2	B	329	ALA	2.2
2	F	363	ALA	2.2
2	H	148	VAL	2.2
2	H	195	TYR	2.2
2	D	55	THR	2.2
2	H	134	ALA	2.2
2	D	167	ILE	2.2
2	D	134	ALA	2.1
1	E	230	ALA	2.1
2	B	373	VAL	2.1
1	C	210	SER	2.1
1	C	81	VAL	2.1
1	C	302	LEU	2.1
1	E	352	GLY	2.1
2	H	363	ALA	2.1
1	E	287	VAL	2.1
2	D	302	LEU	2.1
1	A	127	PHE	2.1
2	H	167	ILE	2.1
2	B	109	LEU	2.1
2	F	411	LEU	2.1
1	C	363	ALA	2.1
1	E	109	LEU	2.0
2	D	47	LEU	2.0
1	E	289	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	107	LEU	2.0
1	C	283	LEU	2.0
1	A	182	SER	2.0

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, 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	V44	B	203	20/21	0.89	0.20	91,112,114,114	0
2	V44	D	203	20/21	0.89	0.25	93,108,110,111	0
2	V44	F	203	20/21	0.90	0.21	83,104,107,107	0
2	V44	H	203	20/21	0.90	0.18	82,101,102,102	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, 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
3	ZN	A	605	1/1	0.76	0.15	109,109,109,109	0
3	ZN	H	607	1/1	0.83	0.17	104,104,104,104	0
3	ZN	F	600	1/1	0.86	0.10	109,109,109,109	0
3	ZN	A	601	1/1	0.88	0.16	69,69,69,69	0
3	ZN	F	606	1/1	0.89	0.20	133,133,133,133	0
3	ZN	D	600	1/1	0.91	0.08	110,110,110,110	0
3	ZN	F	604	1/1	0.92	0.07	93,93,93,93	0
4	SO4	C	605	5/5	0.93	0.16	77,77,78,78	0
3	ZN	D	605	1/1	0.94	0.16	108,108,108,108	0
3	ZN	C	602	1/1	0.94	0.15	92,92,92,92	0
3	ZN	B	600	1/1	0.94	0.09	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	606	1/1	0.95	0.13	88,88,88,88	0
3	ZN	F	603	1/1	0.96	0.12	100,100,100,100	0
3	ZN	D	603	1/1	0.96	0.12	77,77,77,77	0
3	ZN	E	604	1/1	0.96	0.17	78,78,78,78	0
3	ZN	H	603	1/1	0.96	0.20	110,110,110,110	0
3	ZN	H	604	1/1	0.96	0.14	95,95,95,95	0
3	ZN	E	606	1/1	0.96	0.17	120,120,120,120	0
3	ZN	B	602	1/1	0.96	0.15	82,82,82,82	0
3	ZN	A	603	1/1	0.97	0.11	86,86,86,86	0
3	ZN	E	603	1/1	0.97	0.15	57,57,57,57	0
3	ZN	C	601	1/1	0.97	0.17	68,68,68,68	0
3	ZN	G	601	1/1	0.97	0.11	85,85,85,85	0
3	ZN	H	601	1/1	0.97	0.19	71,71,71,71	0
3	ZN	H	602	1/1	0.97	0.18	85,85,85,85	0
3	ZN	E	605	1/1	0.97	0.14	101,101,101,101	0
3	ZN	D	604	1/1	0.97	0.17	60,60,60,60	0
3	ZN	H	606	1/1	0.97	0.13	71,71,71,71	0
3	ZN	A	604	1/1	0.97	0.09	111,111,111,111	0
3	ZN	F	602	1/1	0.97	0.11	89,89,89,89	0
3	ZN	F	601	1/1	0.98	0.17	63,63,63,63	0
3	ZN	A	602	1/1	0.98	0.11	88,88,88,88	0
3	ZN	C	500	1/1	0.98	0.16	60,60,60,60	0
3	ZN	B	500	1/1	0.98	0.19	61,61,61,61	0
3	ZN	F	605	1/1	0.98	0.12	113,113,113,113	0
3	ZN	B	501	1/1	0.98	0.19	60,60,60,60	0
3	ZN	G	500	1/1	0.98	0.18	59,59,59,59	0
3	ZN	E	500	1/1	0.98	0.17	63,63,63,63	0
3	ZN	H	600	1/1	0.98	0.07	104,104,104,104	0
3	ZN	E	602	1/1	0.98	0.14	61,61,61,61	0
3	ZN	C	603	1/1	0.98	0.16	85,85,85,85	0
3	ZN	B	601	1/1	0.98	0.14	73,73,73,73	0
3	ZN	D	500	1/1	0.98	0.18	64,64,64,64	0
3	ZN	H	605	1/1	0.98	0.06	89,89,89,89	0
3	ZN	D	601	1/1	0.98	0.18	63,63,63,63	0
3	ZN	D	602	1/1	0.98	0.18	61,61,61,61	0
4	SO4	C	604	5/5	0.98	0.19	56,56,57,58	0
3	ZN	F	500	1/1	0.98	0.17	56,56,56,56	0
3	ZN	A	501	1/1	0.99	0.18	55,55,55,55	0
3	ZN	D	501	1/1	0.99	0.11	66,66,66,66	0
3	ZN	C	501	1/1	0.99	0.15	58,58,58,58	0
3	ZN	H	500	1/1	0.99	0.16	58,58,58,58	0
3	ZN	H	501	1/1	0.99	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	F	501	1/1	0.99	0.17	52,52,52,52	0
3	ZN	E	601	1/1	0.99	0.15	72,72,72,72	0
3	ZN	E	501	1/1	1.00	0.18	63,63,63,63	0
3	ZN	G	501	1/1	1.00	0.15	61,61,61,61	0
3	ZN	A	500	1/1	1.00	0.19	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.