



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:09 PM UTC

PDB ID : 2GWC / pdb_00002gwc
Title : Crystal structure of plant glutamate cysteine ligase in complex with a transition state analogue
Authors : Hothorn, M.; Wachter, A.; Gromes, R.; Stuwe, T.; Rausch, T.; Scheffzek, K.
Deposited on : 2006-05-04
Resolution : 2.18 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

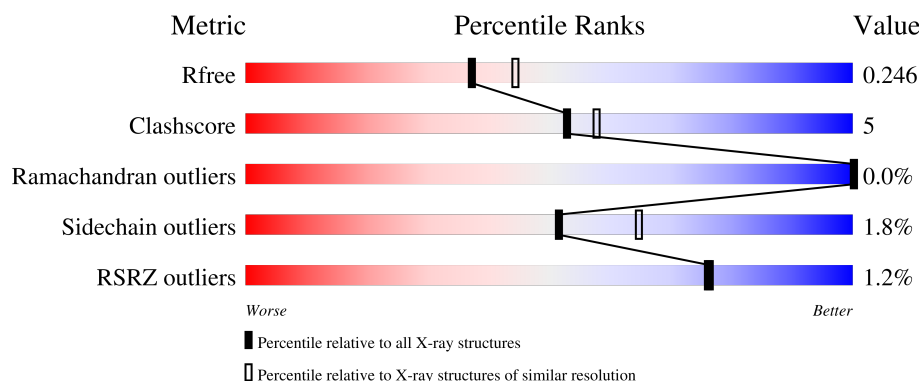
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	449	% 88% 9% .
1	B	449	% 87% 10% .
1	C	449	90% 6% ..
1	D	449	2% 87% 10% .
1	E	449	% 88% 8% ..

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Mol	Chain	Length	Quality of chain
1	F	449	% 87% 10% ..
1	G	449	2% 87% 10% ..
1	H	449	% 86% 10% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 29207 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 Glutamate cysteine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	1	0
			3509	2248	591	646	6	18			
1	B	436	Total	C	N	O	S	Se	0	1	0
			3500	2242	589	645	6	18			
1	C	436	Total	C	N	O	S	Se	0	1	0
			3500	2242	589	645	6	18			
1	D	438	Total	C	N	O	S	Se	0	3	0
			3526	2258	595	649	6	18			
1	E	436	Total	C	N	O	S	Se	0	2	0
			3506	2247	590	645	6	18			
1	F	439	Total	C	N	O	S	Se	0	1	0
			3517	2252	592	649	6	18			
1	G	438	Total	C	N	O	S	Se	0	1	0
			3512	2249	591	648	6	18			
1	H	436	Total	C	N	O	S	Se	0	1	0
			3500	2242	589	645	6	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MSE	MET	modified residue	UNP O23736
A	141	MSE	MET	modified residue	UNP O23736
A	195	MSE	MET	modified residue	UNP O23736
A	202	MSE	MET	modified residue	UNP O23736
A	216	MSE	MET	modified residue	UNP O23736
A	224	MSE	MET	modified residue	UNP O23736
A	228	MSE	MET	modified residue	UNP O23736
A	238	MSE	MET	modified residue	UNP O23736
A	239	MSE	MET	modified residue	UNP O23736
A	257	MSE	MET	modified residue	UNP O23736
A	291	MSE	MET	modified residue	UNP O23736
A	306	MSE	MET	modified residue	UNP O23736
A	329	MSE	MET	modified residue	UNP O23736

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Chain	Residue	Modelled	Actual	Comment	Reference
A	344	MSE	MET	modified residue	UNP O23736
A	384	MSE	MET	modified residue	UNP O23736
A	386	MSE	MET	modified residue	UNP O23736
A	431	MSE	MET	modified residue	UNP O23736
A	496	MSE	MET	modified residue	UNP O23736
B	119	MSE	MET	modified residue	UNP O23736
B	141	MSE	MET	modified residue	UNP O23736
B	195	MSE	MET	modified residue	UNP O23736
B	202	MSE	MET	modified residue	UNP O23736
B	216	MSE	MET	modified residue	UNP O23736
B	224	MSE	MET	modified residue	UNP O23736
B	228	MSE	MET	modified residue	UNP O23736
B	238	MSE	MET	modified residue	UNP O23736
B	239	MSE	MET	modified residue	UNP O23736
B	257	MSE	MET	modified residue	UNP O23736
B	291	MSE	MET	modified residue	UNP O23736
B	306	MSE	MET	modified residue	UNP O23736
B	329	MSE	MET	modified residue	UNP O23736
B	344	MSE	MET	modified residue	UNP O23736
B	384	MSE	MET	modified residue	UNP O23736
B	386	MSE	MET	modified residue	UNP O23736
B	431	MSE	MET	modified residue	UNP O23736
B	496	MSE	MET	modified residue	UNP O23736
C	119	MSE	MET	modified residue	UNP O23736
C	141	MSE	MET	modified residue	UNP O23736
C	195	MSE	MET	modified residue	UNP O23736
C	202	MSE	MET	modified residue	UNP O23736
C	216	MSE	MET	modified residue	UNP O23736
C	224	MSE	MET	modified residue	UNP O23736
C	228	MSE	MET	modified residue	UNP O23736
C	238	MSE	MET	modified residue	UNP O23736
C	239	MSE	MET	modified residue	UNP O23736
C	257	MSE	MET	modified residue	UNP O23736
C	291	MSE	MET	modified residue	UNP O23736
C	306	MSE	MET	modified residue	UNP O23736
C	329	MSE	MET	modified residue	UNP O23736
C	344	MSE	MET	modified residue	UNP O23736
C	384	MSE	MET	modified residue	UNP O23736
C	386	MSE	MET	modified residue	UNP O23736
C	431	MSE	MET	modified residue	UNP O23736
C	496	MSE	MET	modified residue	UNP O23736
D	119	MSE	MET	modified residue	UNP O23736

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Chain	Residue	Modelled	Actual	Comment	Reference
D	141	MSE	MET	modified residue	UNP O23736
D	195	MSE	MET	modified residue	UNP O23736
D	202	MSE	MET	modified residue	UNP O23736
D	216	MSE	MET	modified residue	UNP O23736
D	224	MSE	MET	modified residue	UNP O23736
D	228	MSE	MET	modified residue	UNP O23736
D	238	MSE	MET	modified residue	UNP O23736
D	239	MSE	MET	modified residue	UNP O23736
D	257	MSE	MET	modified residue	UNP O23736
D	291	MSE	MET	modified residue	UNP O23736
D	306	MSE	MET	modified residue	UNP O23736
D	329	MSE	MET	modified residue	UNP O23736
D	344	MSE	MET	modified residue	UNP O23736
D	384	MSE	MET	modified residue	UNP O23736
D	386	MSE	MET	modified residue	UNP O23736
D	431	MSE	MET	modified residue	UNP O23736
D	496	MSE	MET	modified residue	UNP O23736
E	119	MSE	MET	modified residue	UNP O23736
E	141	MSE	MET	modified residue	UNP O23736
E	195	MSE	MET	modified residue	UNP O23736
E	202	MSE	MET	modified residue	UNP O23736
E	216	MSE	MET	modified residue	UNP O23736
E	224	MSE	MET	modified residue	UNP O23736
E	228	MSE	MET	modified residue	UNP O23736
E	238	MSE	MET	modified residue	UNP O23736
E	239	MSE	MET	modified residue	UNP O23736
E	257	MSE	MET	modified residue	UNP O23736
E	291	MSE	MET	modified residue	UNP O23736
E	306	MSE	MET	modified residue	UNP O23736
E	329	MSE	MET	modified residue	UNP O23736
E	344	MSE	MET	modified residue	UNP O23736
E	384	MSE	MET	modified residue	UNP O23736
E	386	MSE	MET	modified residue	UNP O23736
E	431	MSE	MET	modified residue	UNP O23736
E	496	MSE	MET	modified residue	UNP O23736
F	119	MSE	MET	modified residue	UNP O23736
F	141	MSE	MET	modified residue	UNP O23736
F	195	MSE	MET	modified residue	UNP O23736
F	202	MSE	MET	modified residue	UNP O23736
F	216	MSE	MET	modified residue	UNP O23736
F	224	MSE	MET	modified residue	UNP O23736
F	228	MSE	MET	modified residue	UNP O23736

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Chain	Residue	Modelled	Actual	Comment	Reference
F	238	MSE	MET	modified residue	UNP O23736
F	239	MSE	MET	modified residue	UNP O23736
F	257	MSE	MET	modified residue	UNP O23736
F	291	MSE	MET	modified residue	UNP O23736
F	306	MSE	MET	modified residue	UNP O23736
F	329	MSE	MET	modified residue	UNP O23736
F	344	MSE	MET	modified residue	UNP O23736
F	384	MSE	MET	modified residue	UNP O23736
F	386	MSE	MET	modified residue	UNP O23736
F	431	MSE	MET	modified residue	UNP O23736
F	496	MSE	MET	modified residue	UNP O23736
G	119	MSE	MET	modified residue	UNP O23736
G	141	MSE	MET	modified residue	UNP O23736
G	195	MSE	MET	modified residue	UNP O23736
G	202	MSE	MET	modified residue	UNP O23736
G	216	MSE	MET	modified residue	UNP O23736
G	224	MSE	MET	modified residue	UNP O23736
G	228	MSE	MET	modified residue	UNP O23736
G	238	MSE	MET	modified residue	UNP O23736
G	239	MSE	MET	modified residue	UNP O23736
G	257	MSE	MET	modified residue	UNP O23736
G	291	MSE	MET	modified residue	UNP O23736
G	306	MSE	MET	modified residue	UNP O23736
G	329	MSE	MET	modified residue	UNP O23736
G	344	MSE	MET	modified residue	UNP O23736
G	384	MSE	MET	modified residue	UNP O23736
G	386	MSE	MET	modified residue	UNP O23736
G	431	MSE	MET	modified residue	UNP O23736
G	496	MSE	MET	modified residue	UNP O23736
H	119	MSE	MET	modified residue	UNP O23736
H	141	MSE	MET	modified residue	UNP O23736
H	195	MSE	MET	modified residue	UNP O23736
H	202	MSE	MET	modified residue	UNP O23736
H	216	MSE	MET	modified residue	UNP O23736
H	224	MSE	MET	modified residue	UNP O23736
H	228	MSE	MET	modified residue	UNP O23736
H	238	MSE	MET	modified residue	UNP O23736
H	239	MSE	MET	modified residue	UNP O23736
H	257	MSE	MET	modified residue	UNP O23736
H	291	MSE	MET	modified residue	UNP O23736
H	306	MSE	MET	modified residue	UNP O23736
H	329	MSE	MET	modified residue	UNP O23736

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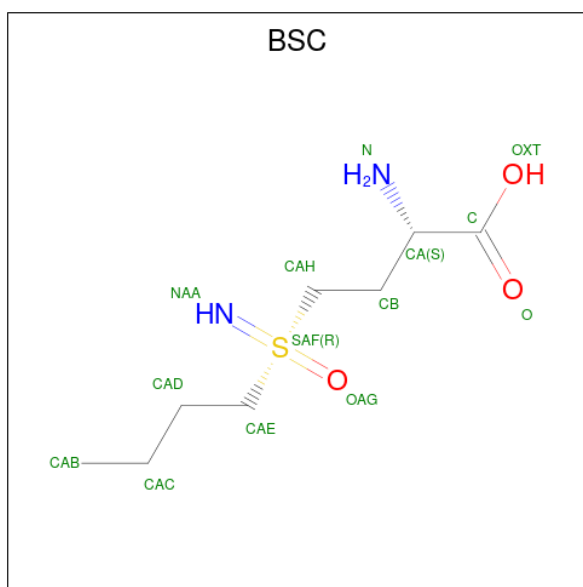
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Chain	Residue	Modelled	Actual	Comment	Reference
H	344	MSE	MET	modified residue	UNP O23736
H	384	MSE	MET	modified residue	UNP O23736
H	386	MSE	MET	modified residue	UNP O23736
H	431	MSE	MET	modified residue	UNP O23736
H	496	MSE	MET	modified residue	UNP O23736

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is (2S)-2-amino-4-(S-butylsulfonimidoyl)butanoic acid (CCD ID: BSC) (formula: C₈H₁₈N₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	B	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	C	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	D	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	E	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	F	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	G	1	Total	C	N	O	S	0	0
			14	8	2	3	1		
3	H	1	Total	C	N	O	S	0	0
			14	8	2	3	1		

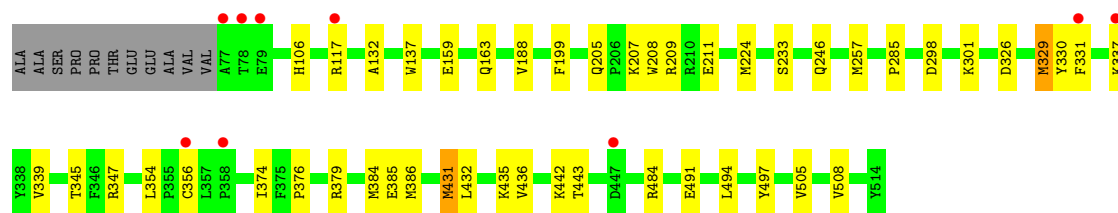
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		
4	B	128	Total	O	0	0
			128	128		
4	C	124	Total	O	0	0
			124	124		
4	D	120	Total	O	0	0
			120	120		

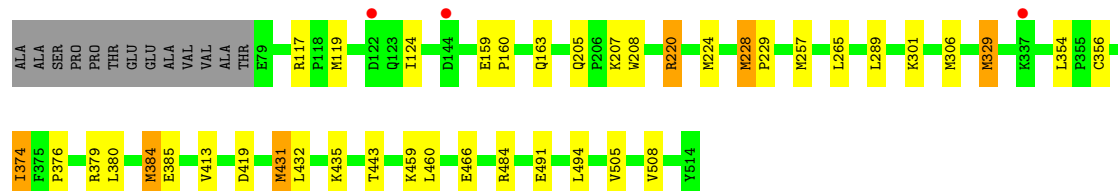
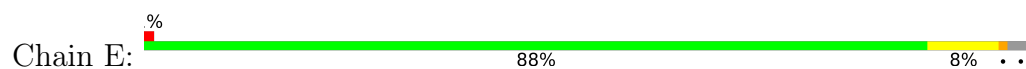
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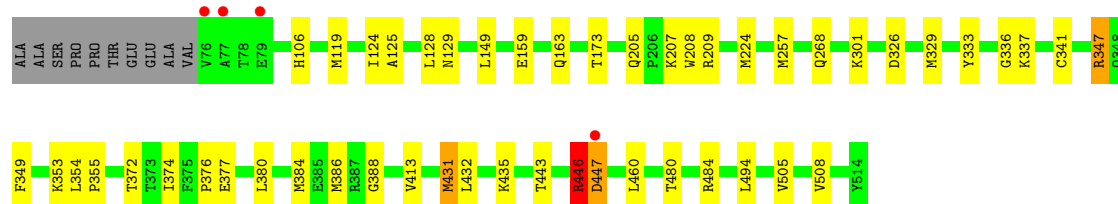
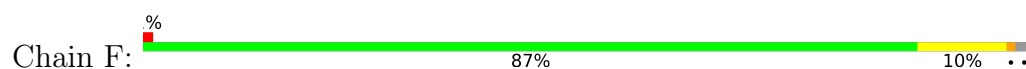
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	138	Total 138	O 138	0	0
4	F	119	Total 119	O 119	0	0
4	G	130	Total 130	O 130	0	0
4	H	107	Total 107	O 107	0	0



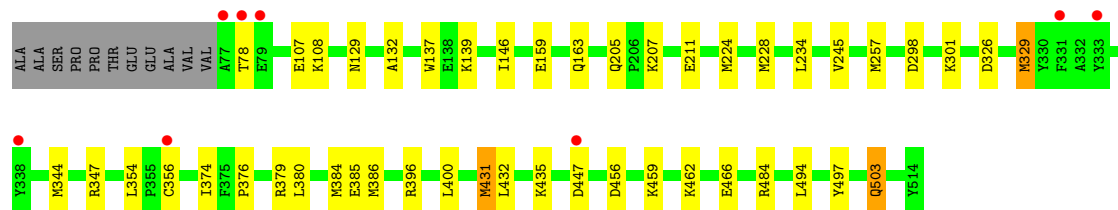
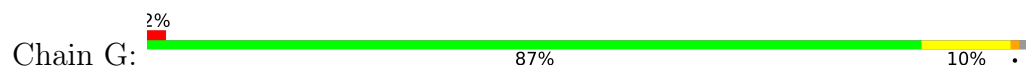
• Molecule 1: Glutamate cysteine ligase



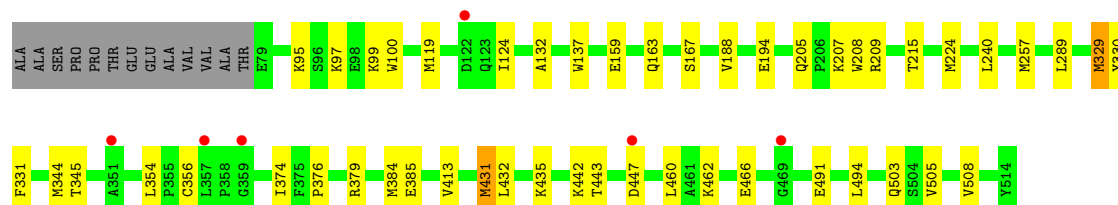
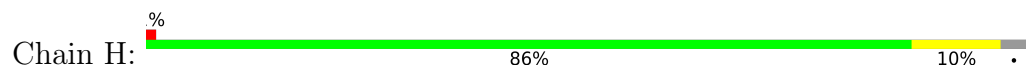
• Molecule 1: Glutamate cysteine ligase



• Molecule 1: Glutamate cysteine ligase



• Molecule 1: Glutamate cysteine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.04Å 198.92Å 114.97Å 90.00° 99.66° 90.00°	Depositor
Resolution (Å)	99.50 – 2.18 99.50 – 2.18	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.50-2.18) 97.5 (99.50-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	146.93 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.241 0.205 , 0.246	Depositor DCC
R_{free} test set	9951 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29207	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1499e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BSC, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	1/3580 (0.0%)	0.94	1/4812 (0.0%)
1	B	0.83	1/3571 (0.0%)	0.89	0/4799
1	C	0.85	1/3571 (0.0%)	0.91	1/4799 (0.0%)
1	D	0.88	2/3603 (0.1%)	0.92	0/4843
1	E	0.89	3/3580 (0.1%)	0.91	0/4810
1	F	0.85	0/3588	0.89	1/4823 (0.0%)
1	G	0.89	3/3583 (0.1%)	0.94	0/4816
1	H	0.85	3/3571 (0.1%)	0.91	0/4799
All	All	0.87	14/28647 (0.0%)	0.91	3/38501 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	MSE	SE-CE	-8.26	1.70	1.95
1	D	329	MSE	SE-CE	-7.83	1.72	1.95
1	H	329	MSE	SE-CE	-7.29	1.73	1.95
1	E	329	MSE	SE-CE	-6.43	1.76	1.95
1	E	228	MSE	SE-CE	6.00	2.13	1.95
1	E	374	ILE	CA-CB	5.86	1.61	1.54
1	C	329	MSE	SE-CE	-5.77	1.78	1.95
1	A	195	MSE	SE-CE	5.65	2.12	1.95
1	G	329	MSE	SE-CE	-5.47	1.79	1.95
1	G	146	ILE	CA-CB	5.30	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	188	VAL	CA-CB	5.24	1.60	1.54
1	D	339	VAL	CA-CB	5.11	1.60	1.54
1	H	447	ASP	CG-OD2	5.04	1.34	1.25
1	G	447	ASP	CG-OD2	5.04	1.34	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	356	CYS	N-CA-C	6.91	118.89	111.36
1	A	337	LYS	N-CA-C	6.14	118.51	109.24
1	F	337	LYS	N-CA-C	5.00	116.80	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	388	GLY	Peptide
1	F	447	ASP	Peptide

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	3509	0	3461	32	0
1	B	3500	0	3451	35	0
1	C	3500	0	3451	26	0
1	D	3526	0	3484	38	0
1	E	3506	0	3464	39	0
1	F	3517	0	3465	36	0
1	G	3512	0	3463	38	0
1	H	3500	0	3451	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	14	0	16	1	0
3	B	14	0	16	1	0
3	C	14	0	16	1	0
3	D	14	0	16	1	0
3	E	14	0	16	1	0
3	F	14	0	16	1	0
3	G	14	0	16	3	0
3	H	14	0	16	3	0
4	A	151	0	0	2	0
4	B	128	0	0	3	0
4	C	124	0	0	1	0
4	D	120	0	0	1	0
4	E	138	0	0	6	0
4	F	119	0	0	2	0
4	G	130	0	0	6	0
4	H	107	0	0	5	0
All	All	29207	0	27818	282	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 5.

All (282) 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:329:MSE:HE1	1:C:354:LEU:HD21	1.18	1.18
1:E:329:MSE:HE1	1:E:354:LEU:HD21	1.19	1.12
1:B:329:MSE:HE1	1:B:354:LEU:HD21	1.26	1.09
1:H:329:MSE:HE1	1:H:354:LEU:HD21	1.27	1.09
1:B:329:MSE:CE	1:B:354:LEU:HD21	1.89	1.02
1:H:329:MSE:CE	1:H:354:LEU:HD21	1.89	1.01
1:E:329:MSE:CE	1:E:354:LEU:HD21	1.93	0.98
1:C:329:MSE:CE	1:C:354:LEU:HD21	1.94	0.98
1:D:329:MSE:CE	1:D:354:LEU:HD21	1.94	0.98
1:C:435:LYS:HD3	4:C:535:HOH:O	1.64	0.97
1:E:435:LYS:HD3	4:E:558:HOH:O	1.64	0.97
1:B:431:MSE:HE3	1:B:435:LYS:HD2	1.49	0.94
1:D:329:MSE:HE1	1:D:354:LEU:HD21	1.46	0.94
1:G:329:MSE:HE1	1:G:354:LEU:HD21	1.50	0.91
1:E:257:MSE:HG2	1:E:384:MSE:HE1	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:MSE:HE1	1:A:354:LEU:HD21	1.55	0.88
1:C:431:MSE:HE3	1:C:435:LYS:HD2	1.54	0.87
1:E:431:MSE:HE3	1:E:435:LYS:HD2	1.56	0.86
1:E:329:MSE:HE1	1:E:354:LEU:CD2	2.04	0.85
1:A:447:ASP:CB	1:F:129:ASN:OD1	2.25	0.84
1:C:329:MSE:HE1	1:C:354:LEU:CD2	2.04	0.84
1:H:329:MSE:HE1	1:H:354:LEU:CD2	2.07	0.84
1:B:329:MSE:HE1	1:B:354:LEU:CD2	2.08	0.84
1:A:329:MSE:HE1	1:A:354:LEU:CD2	2.09	0.82
1:G:329:MSE:CE	1:G:354:LEU:HD21	2.09	0.82
1:G:211:GLU:HG3	4:G:595:HOH:O	1.81	0.79
1:B:379:ARG:HD2	1:B:385:GLU:OE2	1.83	0.78
1:G:224:MSE:HE1	3:G:2:BSC:HAC2	1.63	0.78
1:D:224:MSE:HE1	3:D:2:BSC:HAC2	1.66	0.78
1:A:447:ASP:CB	1:F:125:ALA:HB1	2.15	0.76
1:D:329:MSE:HE1	1:D:354:LEU:CD2	2.15	0.75
1:F:431:MSE:HE3	1:F:435:LYS:HD2	1.66	0.75
1:B:257:MSE:HG2	1:B:384:MSE:HE1	1.69	0.74
1:D:431:MSE:HE3	1:D:435:LYS:HD2	1.68	0.74
1:H:354:LEU:HD13	1:H:356:CYS:SG	2.28	0.73
1:A:329:MSE:CE	1:A:354:LEU:HD21	2.18	0.73
1:F:224:MSE:HE1	3:F:2:BSC:HAC2	1.70	0.73
1:G:329:MSE:HE1	1:G:354:LEU:CD2	2.18	0.73
1:A:257:MSE:HG2	1:A:384:MSE:HE1	1.70	0.72
1:D:379:ARG:HD2	1:D:385:GLU:OE2	1.90	0.72
1:H:503:GLN:HG3	4:H:594:HOH:O	1.89	0.71
1:C:431:MSE:HE2	1:C:432:LEU:HA	1.72	0.71
1:H:435:LYS:HD3	4:H:585:HOH:O	1.91	0.71
1:G:456:ASP:O	1:G:459[A]:LYS:HG3	1.91	0.70
1:H:431:MSE:HE3	1:H:435:LYS:HD2	1.73	0.70
1:C:205:GLN:HE21	1:C:207:LYS:H	1.38	0.69
1:B:435:LYS:HD3	4:B:525:HOH:O	1.92	0.69
1:D:329:MSE:HE1	1:D:354:LEU:HD11	1.72	0.69
1:E:205:GLN:HE21	1:E:208:TRP:H	1.40	0.69
1:G:431:MSE:HE3	1:G:435:LYS:CD	2.22	0.69
1:C:257:MSE:HG2	1:C:384:MSE:HE1	1.74	0.69
1:G:431:MSE:HE3	1:G:435:LYS:HD2	1.76	0.68
1:H:95:LYS:HE3	4:H:611:HOH:O	1.93	0.68
1:E:431:MSE:HE2	1:E:432:LEU:HA	1.76	0.67
1:G:205:GLN:HE21	1:G:207:LYS:H	1.42	0.67
1:G:459[A]:LYS:HD2	4:G:534:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MSE:HE3	1:A:124:ILE:HG12	1.76	0.65
1:A:205:GLN:HE21	1:A:207:LYS:H	1.45	0.65
1:G:329:MSE:HE1	1:G:354:LEU:HD11	1.78	0.65
1:D:431:MSE:HE3	1:D:435:LYS:CD	2.26	0.64
1:D:431:MSE:HE2	1:D:432:LEU:HA	1.79	0.64
1:B:431:MSE:HE3	1:B:435:LYS:CD	2.26	0.64
1:A:431:MSE:HE3	1:A:435:LYS:HD2	1.78	0.63
1:C:119:MSE:HE3	1:C:124:ILE:HG12	1.81	0.63
1:G:344:MSE:HE1	4:G:610:HOH:O	1.97	0.63
1:E:379:ARG:HD2	1:E:385:GLU:OE2	1.99	0.63
1:D:257:MSE:HG2	1:D:384:MSE:HE1	1.81	0.63
1:F:431:MSE:HE2	1:F:432:LEU:HA	1.80	0.62
1:H:505:VAL:O	1:H:508:VAL:HG12	1.99	0.62
1:H:205:GLN:HE21	1:H:207:LYS:H	1.48	0.62
1:F:326:ASP:OD1	1:F:347:ARG:NH1	2.32	0.62
1:B:380:LEU:HD13	1:B:384:MSE:HE2	1.81	0.61
1:F:205:GLN:HE21	1:F:208:TRP:H	1.47	0.61
1:F:354:LEU:HB2	4:F:515:HOH:O	2.01	0.61
1:H:431:MSE:HE3	1:H:435:LYS:HB2	1.82	0.61
1:D:209:ARG:HH11	1:D:211:GLU:HG2	1.64	0.61
1:C:224:MSE:HE1	3:C:2:BSC:HAC1	1.83	0.61
1:B:205:GLN:HE21	1:B:207:LYS:H	1.47	0.60
1:E:220:ARG:HD3	4:E:599:HOH:O	2.01	0.59
1:H:431:MSE:HE2	1:H:432:LEU:HA	1.84	0.59
3:G:2:BSC:N	4:G:549:HOH:O	2.32	0.59
1:C:354:LEU:HD13	1:C:356:CYS:SG	2.43	0.59
1:E:354:LEU:HD13	1:E:356:CYS:SG	2.42	0.59
1:G:205:GLN:NE2	1:G:207:LYS:H	1.99	0.59
1:A:431:MSE:HE3	1:A:435:LYS:CD	2.32	0.59
1:C:481:GLU:OE2	1:C:484:ARG:NH2	2.27	0.58
1:F:333:TYR:OH	1:F:336:GLY:HA2	2.04	0.58
1:H:431:MSE:HE3	1:H:435:LYS:CD	2.32	0.58
1:A:106:HIS:HD2	4:A:543:HOH:O	1.86	0.58
1:E:380:LEU:HD13	1:E:384:MSE:HE2	1.87	0.57
1:C:380:LEU:HD13	1:C:384:MSE:CE	2.34	0.57
1:F:329:MSE:HE1	1:F:354:LEU:CD2	2.34	0.57
1:F:431:MSE:HE1	1:F:443:THR:CG2	2.35	0.57
1:E:205:GLN:NE2	1:E:207:LYS:H	2.03	0.57
1:E:431:MSE:HE3	1:E:435:LYS:HB2	1.87	0.56
1:E:431:MSE:HE1	1:E:443:THR:CG2	2.35	0.56
1:D:329:MSE:HE2	1:D:354:LEU:HD21	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:379:ARG:HD2	1:H:385:GLU:OE2	2.05	0.56
1:E:435:LYS:CD	4:E:558:HOH:O	2.39	0.56
1:B:354:LEU:HD13	1:B:356:CYS:SG	2.45	0.56
1:G:431:MSE:HE2	1:G:432:LEU:HA	1.88	0.56
1:A:257:MSE:HG2	1:A:384:MSE:CE	2.36	0.55
1:C:379:ARG:HD2	1:C:385:GLU:OE2	2.05	0.55
1:G:356:CYS:HB3	4:G:610:HOH:O	2.07	0.55
1:A:267:LEU:HD22	1:A:270:ILE:HD12	1.89	0.55
1:B:431:MSE:HE2	1:B:432:LEU:HA	1.88	0.55
1:D:205:GLN:HE21	1:D:208:TRP:H	1.54	0.55
1:D:329:MSE:HE1	1:D:354:LEU:CD1	2.36	0.55
1:G:129:ASN:HD22	1:G:139:LYS:NZ	2.05	0.55
1:H:224:MSE:HE1	3:H:2:BSC:HAC2	1.89	0.54
1:D:205:GLN:NE2	1:D:207:LYS:H	2.05	0.54
1:A:205:GLN:NE2	1:A:207:LYS:H	2.04	0.54
1:A:484:ARG:HD3	1:E:466:GLU:HB3	1.90	0.54
1:F:257:MSE:HG2	1:F:384:MSE:HE1	1.88	0.54
1:D:379:ARG:HD2	1:D:385:GLU:CD	2.33	0.53
1:F:329:MSE:HE3	1:F:341:CYS:HB3	1.90	0.53
1:G:329:MSE:HE1	1:G:354:LEU:CD1	2.39	0.53
1:A:431:MSE:HE1	1:A:443:THR:CG2	2.38	0.53
1:B:132:ALA:HA	1:B:137:TRP:HB2	1.89	0.53
1:B:374:ILE:HG22	1:B:376:PRO:HD3	1.89	0.53
1:A:205:GLN:HE21	1:A:208:TRP:H	1.56	0.53
1:H:205:GLN:HE21	1:H:208:TRP:H	1.57	0.53
1:A:129:ASN:OD1	1:A:139:LYS:NZ	2.24	0.52
1:E:119:MSE:HE3	1:E:124:ILE:HG12	1.91	0.52
1:F:431:MSE:HE3	1:F:435:LYS:HB2	1.90	0.52
1:D:326:ASP:OD1	1:D:347:ARG:NH1	2.42	0.52
1:H:205:GLN:NE2	1:H:207:LYS:H	2.05	0.52
1:H:431:MSE:HE1	1:H:443:THR:CG2	2.40	0.52
1:A:224:MSE:HE1	3:A:2:BSC:HAC1	1.91	0.51
1:F:431:MSE:HE3	1:F:435:LYS:CD	2.37	0.51
1:D:379:ARG:CD	1:D:385:GLU:OE2	2.59	0.51
1:D:354:LEU:HD13	1:D:356:CYS:SG	2.50	0.51
1:C:330:TYR:HB3	1:C:331:PHE:CD2	2.45	0.51
1:G:159:GLU:HB2	1:G:163:GLN:HB2	1.92	0.51
1:C:413:VAL:HG13	1:C:460:LEU:HB3	1.92	0.51
1:H:132:ALA:HA	1:H:137:TRP:HB2	1.92	0.50
1:E:205:GLN:HE21	1:E:207:LYS:H	1.58	0.50
1:F:329:MSE:HE1	1:F:354:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:431:MSE:CE	1:F:435:LYS:HB2	2.42	0.50
1:G:257:MSE:HG2	1:G:384:MSE:HE1	1.93	0.50
1:D:209:ARG:HH11	1:D:211:GLU:CG	2.23	0.50
1:G:326:ASP:OD1	1:G:347:ARG:NH1	2.45	0.50
1:G:462:LYS:O	1:G:466:GLU:HG2	2.11	0.50
1:A:374:ILE:HG22	1:A:376:PRO:HD3	1.94	0.50
1:H:119:MSE:HE2	4:H:568:HOH:O	2.12	0.50
1:D:432:LEU:O	1:D:436:VAL:HG23	2.12	0.50
1:G:107:GLU:OE1	3:G:2:BSC:N	2.44	0.49
1:F:380:LEU:HD13	1:F:384:MSE:HE2	1.94	0.49
1:H:257:MSE:HG2	1:H:384:MSE:HE1	1.94	0.49
1:B:205:GLN:NE2	1:B:207:LYS:H	2.11	0.49
1:D:374:ILE:HG22	1:D:376:PRO:HD3	1.93	0.49
1:H:431:MSE:CE	1:H:435:LYS:HB2	2.43	0.49
1:A:380:LEU:HD13	1:A:384:MSE:HE2	1.95	0.49
1:D:233:SER:OG	1:D:298:ASP:OD2	2.31	0.48
1:H:374:ILE:HG22	1:H:376:PRO:HD3	1.95	0.48
1:C:132:ALA:HA	1:C:137:TRP:HB2	1.95	0.48
1:C:431:MSE:HE2	1:C:432:LEU:CA	2.42	0.48
1:E:435:LYS:CE	4:E:558:HOH:O	2.59	0.48
1:E:435:LYS:HE2	4:E:558:HOH:O	2.14	0.48
1:A:431:MSE:HE2	1:A:432:LEU:HA	1.96	0.48
1:C:431:MSE:HE1	1:C:443:THR:CG2	2.44	0.48
1:G:396:ARG:NH2	4:G:579:HOH:O	2.26	0.47
1:H:329:MSE:HE1	1:H:354:LEU:CG	2.44	0.47
1:A:119:MSE:HE2	4:A:525:HOH:O	2.13	0.47
1:D:209:ARG:NH1	1:D:211:GLU:HG2	2.28	0.47
1:F:374:ILE:HG22	1:F:376:PRO:HD3	1.97	0.47
1:H:431:MSE:HE2	1:H:431:MSE:C	2.39	0.47
1:A:431:MSE:CE	1:A:435:LYS:HB2	2.45	0.47
1:D:188:VAL:CG1	1:D:199:PHE:CE2	2.98	0.47
1:E:431:MSE:HE3	1:E:435:LYS:CB	2.45	0.47
1:G:129:ASN:HD22	1:G:139:LYS:HZ3	1.61	0.47
1:B:248:ASN:OD1	1:B:385:GLU:HG2	2.15	0.47
1:B:458:LEU:HD22	1:B:483:VAL:HG21	1.97	0.47
1:D:132:ALA:HA	1:D:137:TRP:HB2	1.97	0.47
1:B:159:GLU:HB2	1:B:163:GLN:HB2	1.97	0.47
1:F:329:MSE:HE1	1:F:354:LEU:HD21	1.96	0.47
1:F:384:MSE:HG2	1:F:386:MSE:CE	2.45	0.47
1:E:119:MSE:HG2	1:E:124:ILE:HG13	1.97	0.47
1:G:132:ALA:HA	1:G:137:TRP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:MSE:HG2	1:G:384:MSE:CE	2.46	0.46
1:G:379:ARG:HD2	1:G:385:GLU:CD	2.40	0.46
1:E:265:LEU:O	1:E:306:MSE:HE1	2.15	0.46
1:H:442:LYS:NZ	1:H:491:GLU:OE1	2.48	0.46
1:F:106:HIS:HD2	4:F:544:HOH:O	1.98	0.46
1:F:128:LEU:HD22	1:F:149:LEU:HG	1.97	0.46
1:G:374:ILE:HG22	1:G:376:PRO:HD3	1.98	0.46
1:B:80:PRO:HA	4:B:570:HOH:O	2.16	0.46
1:F:480:THR:O	1:F:484:ARG:HB2	2.16	0.46
1:B:129:ASN:ND2	1:B:139:LYS:NZ	2.64	0.45
1:B:107:GLU:OE1	3:B:2:BSC:N	2.49	0.45
1:G:354:LEU:HD13	1:G:356:CYS:SG	2.57	0.45
1:D:442:LYS:NZ	1:D:491:GLU:OE1	2.50	0.45
1:D:329:MSE:CE	1:D:354:LEU:CD2	2.77	0.45
1:E:228:MSE:HB2	1:E:229:PRO:HD3	1.98	0.45
1:D:209:ARG:NH1	1:D:211:GLU:CG	2.80	0.45
1:E:159:GLU:HB2	1:E:163:GLN:HB2	1.99	0.45
1:D:246:GLN:HB2	1:D:386:MSE:O	2.16	0.45
3:H:2:BSC:HAE1	3:H:2:BSC:HAB3	1.71	0.45
1:B:257:MSE:HG2	1:B:384:MSE:CE	2.44	0.45
1:C:384:MSE:HG2	1:C:386:MSE:CE	2.47	0.45
1:F:446:ARG:HB2	1:F:447:ASP:H	1.62	0.44
1:H:224:MSE:HE1	3:H:2:BSC:CAC	2.47	0.44
1:A:413:VAL:HG13	1:A:460:LEU:HB3	2.00	0.44
1:E:379:ARG:HD2	1:E:385:GLU:CD	2.42	0.44
1:F:413:VAL:HG13	1:F:460:LEU:HB3	2.00	0.44
1:H:159:GLU:HB2	1:H:163:GLN:HB2	1.99	0.44
1:H:413:VAL:HG13	1:H:460:LEU:HB3	1.97	0.44
1:B:129:ASN:HD22	1:B:139:LYS:NZ	2.16	0.44
1:F:353:LYS:O	1:F:355:PRO:HD3	2.18	0.44
1:G:224:MSE:O	1:G:228:MSE:HG2	2.18	0.44
1:C:119:MSE:HE3	1:C:124:ILE:CG1	2.47	0.44
1:H:462:LYS:O	1:H:466:GLU:HG2	2.18	0.44
1:H:503:GLN:CG	4:H:594:HOH:O	2.59	0.43
1:D:505:VAL:O	1:D:508:VAL:HG12	2.18	0.43
1:D:159:GLU:HB2	1:D:163:GLN:HB2	2.00	0.43
1:A:431:MSE:HE1	1:A:443:THR:HG21	1.99	0.43
1:F:329:MSE:CE	1:F:354:LEU:HD21	2.48	0.43
1:B:289:LEU:HD22	1:B:491:GLU:HG3	2.00	0.43
1:F:372:THR:O	1:F:372:THR:HG22	2.19	0.43
1:B:379:ARG:CD	1:B:385:GLU:OE2	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:GLN:NE2	1:C:207:LYS:H	2.09	0.43
1:C:379:ARG:CD	1:C:385:GLU:OE2	2.67	0.43
1:B:500:GLU:HG2	4:B:623:HOH:O	2.19	0.43
1:G:503:GLN:HE21	1:G:503:GLN:HB2	1.58	0.43
1:F:326:ASP:CG	1:F:347:ARG:NH1	2.77	0.42
1:F:205:GLN:NE2	1:F:207:LYS:H	2.17	0.42
1:G:497:TYR:CE1	1:G:503:GLN:HG3	2.55	0.42
1:B:413:VAL:HG13	1:B:460:LEU:HB3	2.00	0.42
1:B:431:MSE:HE1	1:B:443:THR:CG2	2.49	0.42
1:E:431:MSE:HE2	1:E:431:MSE:C	2.44	0.42
1:A:159:GLU:HB3	1:A:160:PRO:CD	2.49	0.42
1:B:205:GLN:HE21	1:B:208:TRP:H	1.66	0.42
1:F:505:VAL:O	1:F:508:VAL:HG12	2.19	0.42
1:G:234:LEU:HD12	1:G:298:ASP:HB3	2.01	0.42
1:H:289:LEU:HD22	1:H:491:GLU:HG3	2.00	0.42
1:B:330:TYR:HB3	1:B:331:PHE:CD2	2.54	0.42
1:E:224:MSE:HE1	3:E:2:BSC:HAC1	2.02	0.42
1:E:431:MSE:HE3	1:E:435:LYS:CD	2.40	0.42
1:G:380:LEU:HD13	1:G:384:MSE:HE2	2.01	0.42
1:E:159:GLU:HB3	1:E:160:PRO:CD	2.50	0.42
1:F:159:GLU:HB2	1:F:163:GLN:HB2	2.02	0.42
1:A:132:ALA:HA	1:A:137:TRP:HB2	2.01	0.42
1:C:326:ASP:OD1	1:C:347:ARG:NH1	2.53	0.41
1:G:384:MSE:HG2	1:G:386:MSE:CE	2.50	0.41
1:E:431:MSE:HE2	1:E:432:LEU:CA	2.48	0.41
1:A:119:MSE:HG2	1:A:124:ILE:HG13	2.03	0.41
1:B:79:GLU:HA	1:B:80:PRO:HD2	1.92	0.41
1:D:257:MSE:HG2	1:D:384:MSE:CE	2.49	0.41
1:D:285:PRO:HD3	1:D:497:TYR:CZ	2.56	0.41
1:E:384:MSE:HE3	1:E:384:MSE:HB2	1.84	0.41
1:G:245:VAL:HG13	1:G:400:LEU:HG	2.03	0.41
1:G:354:LEU:HD23	1:G:354:LEU:HA	1.85	0.41
1:A:159:GLU:HB2	1:A:163:GLN:HB2	2.01	0.41
1:B:114:ASN:ND2	1:E:419:ASP:OD2	2.54	0.41
1:B:119:MSE:HG2	1:B:124:ILE:HG13	2.03	0.41
1:D:431:MSE:HE1	1:D:443:THR:CG2	2.51	0.41
1:E:413:VAL:HG13	1:E:460:LEU:HB3	2.02	0.41
1:E:505:VAL:O	1:E:508:VAL:HG12	2.20	0.41
1:H:329:MSE:HE2	1:H:345:THR:O	2.20	0.41
1:E:459[B]:LYS:HG2	4:E:576:HOH:O	2.19	0.41
1:F:349:PHE:HA	1:F:354:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:MSE:HE1	1:B:354:LEU:HD11	2.02	0.41
1:D:330:TYR:HB3	1:D:331:PHE:CD2	2.56	0.41
1:H:329:MSE:HE2	1:H:345:THR:C	2.46	0.41
1:H:330:TYR:HB3	1:H:331:PHE:CD2	2.56	0.41
1:H:215:THR:HG22	1:H:240:LEU:HD21	2.03	0.41
1:H:329:MSE:HE3	1:H:354:LEU:HD21	1.93	0.41
1:E:289:LEU:HD22	1:E:491:GLU:HG3	2.02	0.40
1:G:379:ARG:HD2	1:G:385:GLU:OE2	2.20	0.40
1:H:97:LYS:HA	1:H:100:TRP:CE2	2.56	0.40
1:F:119:MSE:HE3	1:F:124:ILE:HG12	2.03	0.40
1:F:268:GLN:HG2	1:F:377:GLU:HB3	2.02	0.40
1:H:119:MSE:HG2	1:H:124:ILE:HG13	2.04	0.40
1:A:333:TYR:OH	1:A:336:GLY:HA2	2.22	0.40
1:C:372:THR:HG22	1:C:372:THR:O	2.22	0.40
1:E:374:ILE:HG22	1:E:376:PRO:HD3	2.04	0.40
1:A:431:MSE:HE2	1:A:431:MSE:C	2.46	0.40
1:B:108:LYS:HZ1	1:B:184:HIS:CD2	2.39	0.40
1:C:431:MSE:HE3	1:C:435:LYS:HB2	2.03	0.40
1:D:329:MSE:HE2	1:D:345:THR:O	2.22	0.40
1:H:344:MSE:SE	1:H:354:LEU:HD22	2.72	0.40
1:D:106:HIS:HD2	4:D:542:HOH:O	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/449 (97%)	430 (98%)	7 (2%)	0	100	100
1	B	435/449 (97%)	426 (98%)	9 (2%)	0	100	100
1	C	435/449 (97%)	428 (98%)	7 (2%)	0	100	100
1	D	439/449 (98%)	433 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	436/449 (97%)	427 (98%)	9 (2%)	0	100	100
1	F	438/449 (98%)	429 (98%)	8 (2%)	1 (0%)	43	49
1	G	437/449 (97%)	427 (98%)	10 (2%)	0	100	100
1	H	435/449 (97%)	428 (98%)	7 (2%)	0	100	100
All	All	3492/3592 (97%)	3428 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	446	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/364 (103%)	367 (98%)	7 (2%)	50	63
1	B	374/364 (103%)	367 (98%)	7 (2%)	50	63
1	C	374/364 (103%)	368 (98%)	6 (2%)	55	68
1	D	377/364 (104%)	370 (98%)	7 (2%)	50	63
1	E	375/364 (103%)	368 (98%)	7 (2%)	50	63
1	F	375/364 (103%)	368 (98%)	7 (2%)	50	63
1	G	375/364 (103%)	368 (98%)	7 (2%)	50	63
1	H	374/364 (103%)	368 (98%)	6 (2%)	55	68
All	All	2998/2912 (103%)	2944 (98%)	54 (2%)	51	65

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ILE
1	A	209	ARG
1	A	301	LYS

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Mol	Chain	Res	Type
1	A	347	ARG
1	A	411	GLU
1	A	431	MSE
1	A	494	LEU
1	B	167	SER
1	B	220	ARG
1	B	278	SER
1	B	301	LYS
1	B	431	MSE
1	B	484	ARG
1	B	494	LEU
1	C	155	SER
1	C	209	ARG
1	C	301	LYS
1	C	354	LEU
1	C	431	MSE
1	C	494	LEU
1	D	117[A]	ARG
1	D	117[B]	ARG
1	D	301	LYS
1	D	337	LYS
1	D	431	MSE
1	D	484	ARG
1	D	494	LEU
1	E	117	ARG
1	E	220	ARG
1	E	301	LYS
1	E	384	MSE
1	E	431	MSE
1	E	484	ARG
1	E	494	LEU
1	F	173	THR
1	F	209	ARG
1	F	301	LYS
1	F	347	ARG
1	F	431	MSE
1	F	446	ARG
1	F	494	LEU
1	G	78	THR
1	G	108	LYS
1	G	301	LYS
1	G	431	MSE

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Mol	Chain	Res	Type
1	G	484	ARG
1	G	494	LEU
1	G	503	GLN
1	H	99	LYS
1	H	167	SER
1	H	194	GLU
1	H	209	ARG
1	H	431	MSE
1	H	494	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	154	GLN
1	A	205	GLN
1	A	369	ASN
1	A	434	ASN
1	B	106	HIS
1	B	114	ASN
1	B	129	ASN
1	B	151	GLN
1	B	154	GLN
1	B	205	GLN
1	B	369	ASN
1	B	434	ASN
1	B	492	ASN
1	C	106	HIS
1	C	129	ASN
1	C	151	GLN
1	C	154	GLN
1	C	205	GLN
1	C	335	ASN
1	C	369	ASN
1	C	434	ASN
1	D	106	HIS
1	D	129	ASN
1	D	154	GLN
1	D	205	GLN
1	D	335	ASN
1	D	369	ASN
1	D	434	ASN

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Mol	Chain	Res	Type
1	D	498	ASN
1	E	106	HIS
1	E	129	ASN
1	E	151	GLN
1	E	154	GLN
1	E	205	GLN
1	E	335	ASN
1	E	369	ASN
1	E	434	ASN
1	E	492	ASN
1	F	106	HIS
1	F	151	GLN
1	F	154	GLN
1	F	182	ASN
1	F	205	GLN
1	F	369	ASN
1	F	434	ASN
1	F	492	ASN
1	G	106	HIS
1	G	129	ASN
1	G	151	GLN
1	G	205	GLN
1	G	294	HIS
1	G	335	ASN
1	G	369	ASN
1	G	434	ASN
1	G	492	ASN
1	G	503	GLN
1	H	106	HIS
1	H	129	ASN
1	H	151	GLN
1	H	154	GLN
1	H	205	GLN
1	H	335	ASN
1	H	369	ASN
1	H	503	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BSC	A	2	2	9,13,13	1.37	1 (11%)	8,17,17	1.19	1 (12%)
3	BSC	D	2	2	9,13,13	1.46	1 (11%)	8,17,17	0.87	0
3	BSC	C	2	2	9,13,13	0.83	0	8,17,17	1.32	1 (12%)
3	BSC	H	2	2	9,13,13	1.10	1 (11%)	8,17,17	1.44	2 (25%)
3	BSC	F	2	2	9,13,13	1.04	1 (11%)	8,17,17	0.80	0
3	BSC	B	2	2	9,13,13	1.07	1 (11%)	8,17,17	1.23	1 (12%)
3	BSC	G	2	2	9,13,13	0.75	0	8,17,17	1.01	0
3	BSC	E	2	2	9,13,13	1.01	1 (11%)	8,17,17	0.80	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
3	BSC	A	2	2	-	1/13/15/15	-
3	BSC	D	2	2	-	0/13/15/15	-
3	BSC	C	2	2	-	1/13/15/15	-
3	BSC	H	2	2	-	3/13/15/15	-
3	BSC	F	2	2	-	3/13/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BSC	B	2	2	-	1/13/15/15	-
3	BSC	G	2	2	-	3/13/15/15	-
3	BSC	E	2	2	-	1/13/15/15	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	BSC	CB-CAH	-3.65	1.49	1.52
3	D	2	BSC	CB-CAH	-3.55	1.49	1.52
3	E	2	BSC	OXT-C	-2.63	1.22	1.30
3	H	2	BSC	CB-CAH	-2.38	1.50	1.52
3	B	2	BSC	CB-CAH	-2.29	1.50	1.52
3	F	2	BSC	CB-CAH	-2.03	1.50	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	BSC	CAD-CAE-SAF	2.89	118.94	112.02
3	H	2	BSC	CAD-CAE-SAF	2.64	118.36	112.02
3	H	2	BSC	CB-CA-C	-2.18	104.67	110.45
3	C	2	BSC	CB-CAH-SAF	-2.18	109.25	114.10
3	A	2	BSC	CB-CA-C	-2.14	104.77	110.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	BSC	CAC-CAD-CAE-SAF
3	B	2	BSC	CAC-CAD-CAE-SAF
3	E	2	BSC	CAC-CAD-CAE-SAF
3	G	2	BSC	CAC-CAD-CAE-SAF
3	H	2	BSC	CAB-CAC-CAD-CAE
3	H	2	BSC	CAD-CAE-SAF-OAG
3	H	2	BSC	CAD-CAE-SAF-CAH
3	G	2	BSC	O-C-CA-CB
3	G	2	BSC	OXT-C-CA-CB
3	F	2	BSC	OXT-C-CA-CB
3	F	2	BSC	O-C-CA-CB
3	C	2	BSC	CAC-CAD-CAE-SAF
3	F	2	BSC	CAD-CAE-SAF-OAG

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	BSC	1	0
3	D	2	BSC	1	0
3	C	2	BSC	1	0
3	H	2	BSC	3	0
3	F	2	BSC	1	0
3	B	2	BSC	1	0
3	G	2	BSC	3	0
3	E	2	BSC	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, 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	420/449 (93%)	0.03	5 (1%) 76 76	14, 23, 28, 37	1 (0%)
1	B	418/449 (93%)	0.12	4 (0%) 79 79	14, 23, 27, 35	1 (0%)
1	C	418/449 (93%)	0.04	1 (0%) 91 90	14, 23, 27, 36	1 (0%)
1	D	420/449 (93%)	0.19	9 (2%) 63 63	11, 23, 27, 37	3 (0%)
1	E	418/449 (93%)	0.11	3 (0%) 84 83	14, 23, 27, 33	2 (0%)
1	F	421/449 (93%)	0.15	4 (0%) 79 79	14, 23, 28, 39	1 (0%)
1	G	420/449 (93%)	0.21	8 (1%) 66 65	14, 23, 28, 38	1 (0%)
1	H	418/449 (93%)	0.07	6 (1%) 73 73	14, 23, 28, 36	1 (0%)
All	All	3353/3592 (93%)	0.11	40 (1%) 76 76	11, 23, 28, 39	11 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ASP	5.7
1	F	447	ASP	5.0
1	D	77	ALA	3.9
1	F	76	VAL	3.3
1	B	114	ASN	3.2
1	G	338	TYR	3.2
1	D	356	CYS	3.0
1	H	359	GLY	3.0
1	F	77	ALA	2.9
1	A	77	ALA	2.8
1	H	447	ASP	2.7
1	D	331	PHE	2.6
1	F	79	GLU	2.6
1	D	117[A]	ARG	2.6
1	G	333	TYR	2.5
1	C	359	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	447	ASP	2.4
1	G	356	CYS	2.4
1	G	331	PHE	2.4
1	D	78	THR	2.4
1	A	84	GLU	2.4
1	G	78	THR	2.4
1	G	77	ALA	2.3
1	H	469	GLY	2.3
1	E	122	ASP	2.3
1	A	337	LYS	2.3
1	B	120	LYS	2.3
1	A	469	GLY	2.3
1	B	333	TYR	2.1
1	D	337	LYS	2.1
1	E	337	LYS	2.1
1	H	357	LEU	2.1
1	D	79	GLU	2.1
1	E	144	ASP	2.1
1	H	122	ASP	2.1
1	G	79	GLU	2.1
1	D	447	ASP	2.0
1	B	337	LYS	2.0
1	H	351	ALA	2.0
1	D	358	PRO	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MG	D	1	1/1	0.89	0.09	36,36,36,36	0
2	MG	G	1	1/1	0.89	0.09	37,37,37,37	0
2	MG	H	1	1/1	0.89	0.09	38,38,38,38	0
2	MG	F	1	1/1	0.93	0.07	27,27,27,27	0
3	BSC	B	2	14/14	0.93	0.12	29,33,35,35	0
3	BSC	G	2	14/14	0.93	0.11	30,33,34,35	0
2	MG	A	1	1/1	0.94	0.08	28,28,28,28	0
3	BSC	C	2	14/14	0.94	0.11	30,31,32,32	0
3	BSC	A	2	14/14	0.94	0.10	25,27,32,33	0
3	BSC	H	2	14/14	0.94	0.11	26,29,33,33	0
2	MG	E	1	1/1	0.95	0.05	34,34,34,34	0
3	BSC	E	2	14/14	0.95	0.09	29,31,32,34	0
3	BSC	F	2	14/14	0.95	0.09	24,26,30,30	0
2	MG	C	1	1/1	0.95	0.05	28,28,28,28	0
2	MG	B	1	1/1	0.95	0.05	27,27,27,27	0
3	BSC	D	2	14/14	0.96	0.09	28,29,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.