Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:25 am BST

PDB ID	:	5ZHX
Title	:	Crystal structure of SmgGDS-558 and farnesylated RhoA complex
Authors	:	Shimizu, H.; Toma-Fukai, S.; Shimizu, T.
Deposited on	:	2018-03-13
Resolution	:	3.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

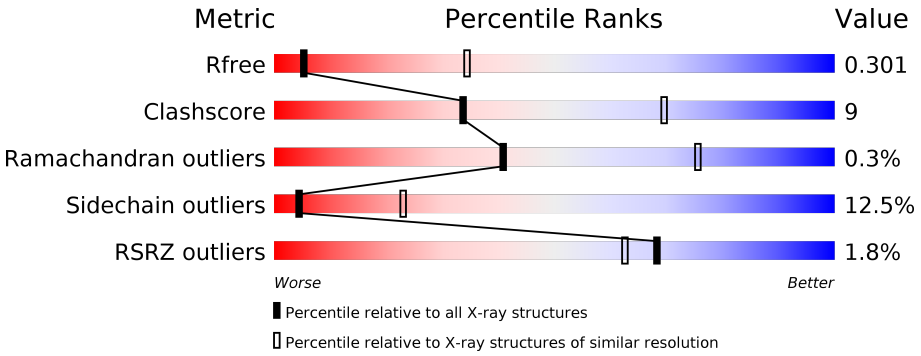
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	487	77% 17%
1	B	487	% 77% 16%
1	C	487	78% 16%
1	D	487	78% 16%
2	e	198	9% 66% 16% 18%
2	f	198	3% 68% 10% 21%

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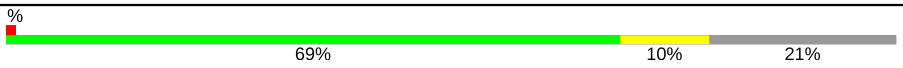
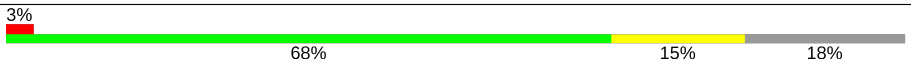
Mol	Chain	Length	Quality of chain
2	g	198	
2	h	198	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18720 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 Rap1 GTPase-GDP dissociation stimulator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3411	2145	595	652	19			
1	B	469	Total	C	N	O	S	0	0	0
			3411	2145	595	652	19			
1	C	469	Total	C	N	O	S	0	0	0
			3411	2145	595	652	19			
1	D	469	Total	C	N	O	S	0	0	0
			3411	2145	595	652	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	GLY	-	expression tag	UNP P52306
A	73	PRO	-	expression tag	UNP P52306
A	74	LEU	-	expression tag	UNP P52306
A	75	GLY	-	expression tag	UNP P52306
A	76	SER	-	expression tag	UNP P52306
B	72	GLY	-	expression tag	UNP P52306
B	73	PRO	-	expression tag	UNP P52306
B	74	LEU	-	expression tag	UNP P52306
B	75	GLY	-	expression tag	UNP P52306
B	76	SER	-	expression tag	UNP P52306
C	72	GLY	-	expression tag	UNP P52306
C	73	PRO	-	expression tag	UNP P52306
C	74	LEU	-	expression tag	UNP P52306
C	75	GLY	-	expression tag	UNP P52306
C	76	SER	-	expression tag	UNP P52306
D	72	GLY	-	expression tag	UNP P52306
D	73	PRO	-	expression tag	UNP P52306
D	74	LEU	-	expression tag	UNP P52306
D	75	GLY	-	expression tag	UNP P52306
D	76	SER	-	expression tag	UNP P52306

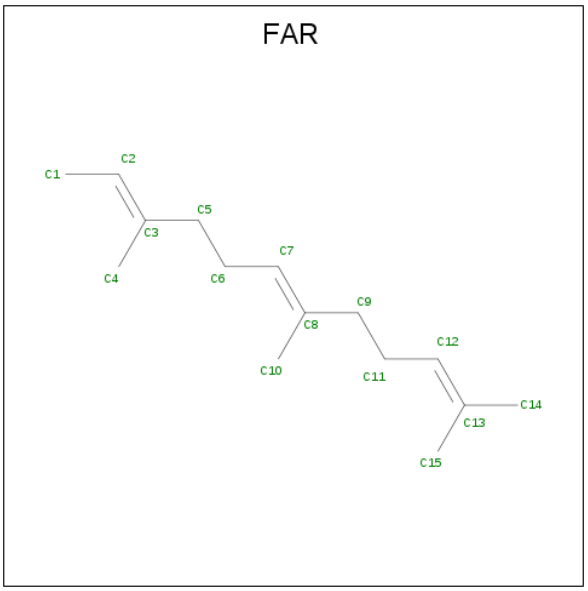
- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	e	163	Total	C	N	O	S	0	0	0
			1288	813	222	242	11			
2	f	156	Total	C	N	O	S	0	0	0
			1220	767	213	231	9			
2	g	156	Total	C	N	O	S	0	0	0
			1220	767	213	231	9			
2	h	163	Total	C	N	O	S	0	0	0
			1288	813	222	242	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-4	GLY	-	expression tag	UNP P61586
e	-3	PRO	-	expression tag	UNP P61586
e	-2	LEU	-	expression tag	UNP P61586
e	-1	GLY	-	expression tag	UNP P61586
e	0	SER	-	expression tag	UNP P61586
e	193	ALA	LEU	engineered mutation	UNP P61586
f	-4	GLY	-	expression tag	UNP P61586
f	-3	PRO	-	expression tag	UNP P61586
f	-2	LEU	-	expression tag	UNP P61586
f	-1	GLY	-	expression tag	UNP P61586
f	0	SER	-	expression tag	UNP P61586
f	193	ALA	LEU	engineered mutation	UNP P61586
g	-4	GLY	-	expression tag	UNP P61586
g	-3	PRO	-	expression tag	UNP P61586
g	-2	LEU	-	expression tag	UNP P61586
g	-1	GLY	-	expression tag	UNP P61586
g	0	SER	-	expression tag	UNP P61586
g	193	ALA	LEU	engineered mutation	UNP P61586
h	-4	GLY	-	expression tag	UNP P61586
h	-3	PRO	-	expression tag	UNP P61586
h	-2	LEU	-	expression tag	UNP P61586
h	-1	GLY	-	expression tag	UNP P61586
h	0	SER	-	expression tag	UNP P61586
h	193	ALA	LEU	engineered mutation	UNP P61586

- Molecule 3 is FARNESYL (three-letter code: FAR) (formula: $C_{15}H_{26}$).



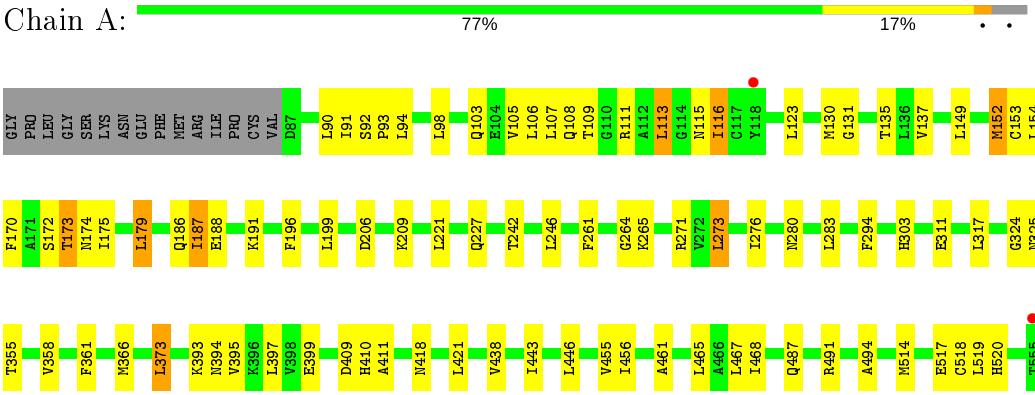
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	e	1	Total C 15 15	0	0
3	f	1	Total C 15 15	0	0
3	g	1	Total C 15 15	0	0
3	h	1	Total C 15 15	0	0

3 Residue-property plots (i)

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

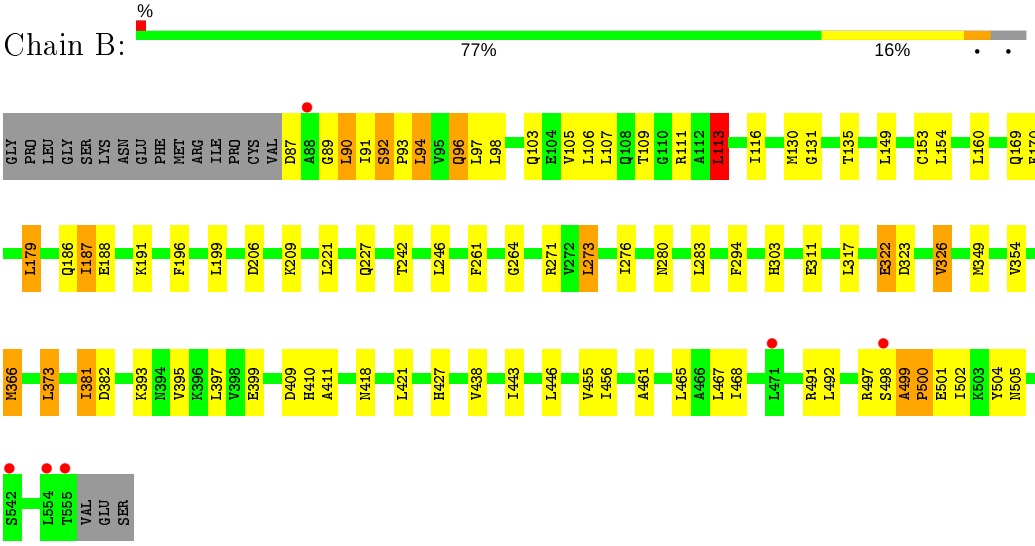
- Molecule 1: Rap1 GTPase-GDP dissociation stimulator 1

Chain A:



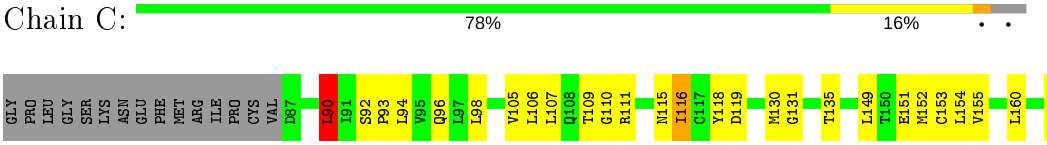
- Molecule 1: Rap1 GTPase-GDP dissociation stimulator 1

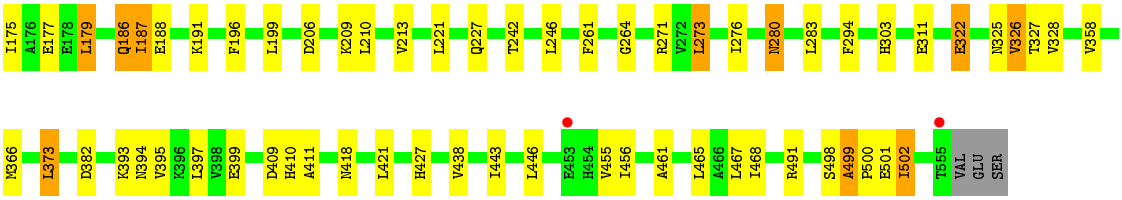
Chain B:



- Molecule 1: Rap1 GTPase-GDP dissociation stimulator 1

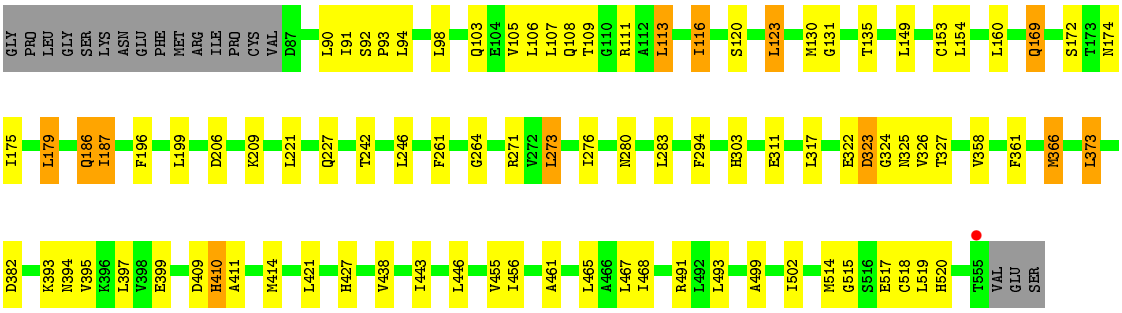
Chain C:





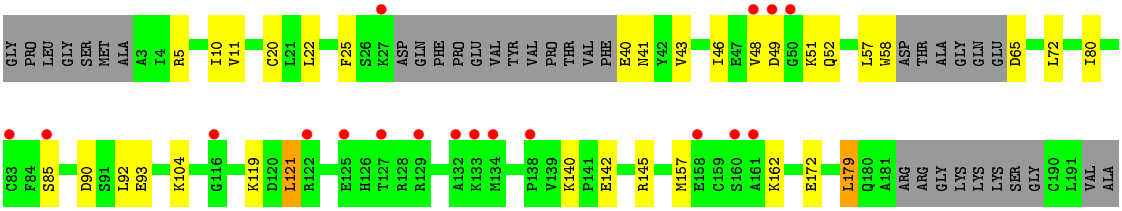
• Molecule 1: Rap1 GTPase-GDP dissociation stimulator 1

Chain D:



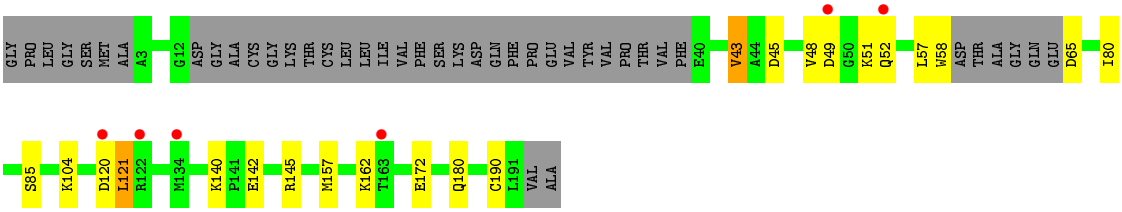
• Molecule 2: Transforming protein RhoA

Chain e:



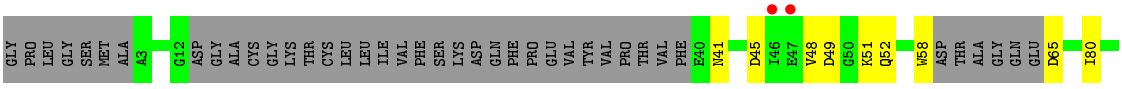
• Molecule 2: Transforming protein RhoA

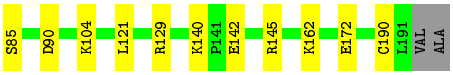
Chain f:



• Molecule 2: Transforming protein RhoA

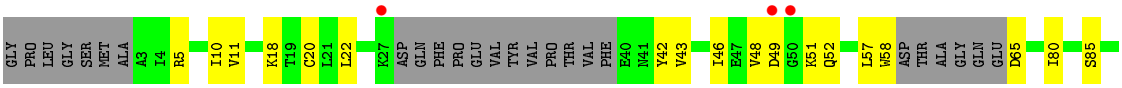
Chain g:

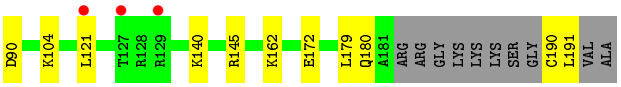




• Molecule 2: Transforming protein RhoA

Chain h:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.32Å 181.77Å 205.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	136.10 – 3.50 25.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (136.10-3.50) 100.0 (25.67-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 3.46Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.250 , 0.306 0.248 , 0.301	Depositor DCC
R_{free} test set	2213 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	113.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 84.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18720	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: FAR

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	0.42	0/3443	0.64	1/4664 (0.0%)
1	B	0.43	0/3443	0.66	2/4664 (0.0%)
1	C	0.42	0/3443	0.64	2/4664 (0.0%)
1	D	0.44	0/3443	0.65	2/4664 (0.0%)
2	e	0.56	1/1308 (0.1%)	0.83	3/1760 (0.2%)
2	f	0.60	2/1240 (0.2%)	0.79	0/1672
2	g	0.58	1/1240 (0.1%)	0.77	0/1672
2	h	0.58	0/1308	0.79	1/1760 (0.1%)
All	All	0.47	4/18868 (0.0%)	0.69	11/25520 (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	A	0	2
1	B	0	2
1	C	0	3
1	D	0	3
2	e	0	1
2	f	0	4
2	g	0	1
All	All	0	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	142	GLU	CD-OE1	6.47	1.32	1.25
2	g	142	GLU	CD-OE1	5.95	1.32	1.25
2	e	142	GLU	CD-OE1	5.41	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	142	GLU	CD-OE2	5.12	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	LEU	CA-CB-CG	6.90	131.17	115.30
1	D	123	LEU	CA-CB-CG	6.87	131.11	115.30
1	B	500	PRO	N-CA-CB	6.46	111.05	103.30
1	B	113	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	113	LEU	CA-CB-CG	5.40	127.71	115.30
2	h	46	ILE	N-CA-C	5.33	125.40	111.00
1	C	500	PRO	N-CA-CB	5.32	109.69	103.30
1	D	113	LEU	CA-CB-CG	5.25	127.38	115.30
2	e	121	LEU	CA-CB-CG	5.17	127.19	115.30
2	e	46	ILE	N-CA-C	5.13	124.86	111.00
2	e	179	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ILE	Peptide
1	A	494	ALA	Peptide
1	B	322	GLU	Peptide
1	B	499	ALA	Peptide
1	C	116	ILE	Peptide
1	C	322	GLU	Peptide
1	C	502	ILE	Peptide
1	D	116	ILE	Peptide
1	D	493	LEU	Peptide
1	D	502	ILE	Peptide
2	e	49	ASP	Peptide
2	f	120	ASP	Peptide
2	f	121	LEU	Peptide
2	f	190	CYS	Peptide
2	f	43	VAL	Peptide
2	g	190	CYS	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	3411	0	3358	47	0
1	B	3411	0	3358	81	0
1	C	3411	0	3358	60	0
1	D	3411	0	3358	47	0
2	e	1288	0	1296	0	0
2	f	1220	0	1201	0	0
2	g	1220	0	1201	0	0
2	h	1288	0	1296	0	0
3	e	15	0	25	0	0
3	f	15	0	25	0	0
3	g	15	0	25	0	0
3	h	15	0	24	0	0
All	All	18720	0	18525	232	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 9.

All (232) 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:325:ASN:ND2	1:C:327:THR:HG22	1.32	1.39
1:C:325:ASN:CG	1:C:327:THR:HG22	1.37	1.39
1:B:186:GLN:OE1	1:B:191:LYS:CG	1.72	1.36
1:A:170:PHE:O	1:A:173:THR:HG22	1.24	1.29
1:C:325:ASN:ND2	1:C:327:THR:CG2	1.96	1.29
1:B:87:ASP:O	1:B:90:LEU:CD2	1.81	1.26
1:B:381:ILE:CD1	1:B:427:HIS:CD2	2.24	1.20
1:A:170:PHE:O	1:A:173:THR:CG2	1.89	1.19
1:B:381:ILE:HD11	1:B:427:HIS:CD2	1.76	1.19
1:B:186:GLN:OE1	1:B:191:LYS:HG2	1.02	1.17
1:C:325:ASN:OD1	1:C:327:THR:HG22	1.45	1.14
1:B:381:ILE:HD11	1:B:427:HIS:HD2	1.08	1.14
1:C:325:ASN:CG	1:C:327:THR:CG2	2.16	1.11
1:C:186:GLN:HG3	1:C:191:LYS:HG2	1.31	1.10
1:D:514:MET:O	1:D:517:GLU:CB	2.00	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASP:O	1:B:90:LEU:HD21	1.47	1.08
1:B:498:SER:HA	1:B:499:ALA:C	1.76	1.03
1:C:325:ASN:HD21	1:C:327:THR:CG2	1.63	1.03
1:B:87:ASP:O	1:B:90:LEU:HD22	1.52	1.02
1:C:186:GLN:CG	1:C:191:LYS:HG2	1.92	1.00
1:D:325:ASN:OD1	1:D:327:THR:HG22	1.61	0.99
1:C:325:ASN:OD1	1:C:327:THR:CG2	2.10	0.98
1:B:381:ILE:CD1	1:B:427:HIS:HD2	1.66	0.97
1:C:186:GLN:HG3	1:C:191:LYS:CG	1.97	0.94
1:C:325:ASN:OD1	1:C:327:THR:N	2.02	0.93
1:C:325:ASN:HD21	1:C:327:THR:HG22	1.16	0.92
1:A:137:VAL:HG11	1:A:173:THR:OG1	1.71	0.90
1:B:90:LEU:H	1:B:90:LEU:HD13	1.37	0.87
1:D:518:CYS:HA	1:D:519:LEU:CB	2.05	0.86
1:A:92:SER:OG	1:A:93:PRO:HD3	1.77	0.84
1:C:92:SER:OG	1:C:93:PRO:HD3	1.77	0.84
1:A:518:CYS:HA	1:A:519:LEU:CB	2.06	0.84
1:D:92:SER:OG	1:D:93:PRO:HD3	1.78	0.84
1:B:381:ILE:O	1:B:381:ILE:HD12	1.78	0.83
1:B:91:ILE:HG21	1:B:130:MET:HE3	1.60	0.83
1:B:89:GLY:O	1:B:93:PRO:HD2	1.80	0.80
1:B:186:GLN:CD	1:B:191:LYS:HG2	2.01	0.78
1:B:91:ILE:HG21	1:B:130:MET:CE	2.14	0.78
1:B:381:ILE:HD12	1:B:381:ILE:C	2.05	0.77
1:C:186:GLN:OE1	1:C:187:ILE:N	2.18	0.77
1:C:325:ASN:ND2	1:C:327:THR:HG21	1.98	0.76
1:A:170:PHE:C	1:A:173:THR:HG22	2.05	0.76
1:B:186:GLN:OE1	1:B:191:LYS:HG3	1.84	0.76
1:C:325:ASN:HD21	1:C:327:THR:HG21	1.50	0.73
1:B:90:LEU:HD23	1:B:91:ILE:HG12	1.73	0.70
1:B:498:SER:CA	1:B:499:ALA:C	2.60	0.69
1:A:169:GLN:O	1:A:172:SER:OG	2.12	0.68
1:A:518:CYS:CB	1:A:520:HIS:N	2.57	0.67
1:D:518:CYS:CB	1:D:520:HIS:N	2.58	0.67
1:B:186:GLN:HE22	1:B:191:LYS:HE2	1.59	0.66
1:C:170:PHE:O	1:C:173:THR:OG1	2.02	0.66
1:D:169:GLN:O	1:D:172:SER:OG	2.14	0.65
1:A:170:PHE:O	1:A:173:THR:HG23	1.91	0.64
1:C:498:SER:N	1:C:499:ALA:HA	2.11	0.64
1:A:514:MET:O	1:A:517:GLU:CB	2.45	0.64
1:B:381:ILE:HD12	1:B:427:HIS:CD2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:ASP:HB2	1:D:410:HIS:HA	1.80	0.63
1:A:409:ASP:HB2	1:A:410:HIS:HA	1.80	0.63
1:C:409:ASP:HB2	1:C:410:HIS:HA	1.79	0.62
1:B:381:ILE:HD13	1:B:427:HIS:CD2	2.32	0.62
1:B:409:ASP:HB2	1:B:410:HIS:HA	1.82	0.61
1:B:170:PHE:O	1:B:173:THR:OG1	2.02	0.61
1:D:325:ASN:CG	1:D:327:THR:HG22	2.22	0.60
1:C:498:SER:H	1:C:499:ALA:HA	1.66	0.60
1:B:498:SER:HA	1:B:499:ALA:O	2.01	0.60
1:B:90:LEU:HD22	1:B:91:ILE:H	1.66	0.60
1:C:382:ASP:O	1:C:427:HIS:CE1	2.56	0.58
1:C:325:ASN:OD1	1:C:327:THR:CA	2.52	0.58
1:D:514:MET:CB	1:D:517:GLU:CB	2.82	0.57
1:A:206:ASP:HA	1:A:209:LYS:HD2	1.86	0.57
1:D:206:ASP:HA	1:D:209:LYS:HD2	1.87	0.57
1:B:206:ASP:HA	1:B:209:LYS:HD2	1.87	0.57
1:B:90:LEU:CD2	1:B:91:ILE:HG12	2.34	0.56
1:B:410:HIS:N	1:B:411:ALA:HA	2.21	0.56
1:A:410:HIS:N	1:A:411:ALA:HA	2.20	0.56
1:B:186:GLN:NE2	1:B:191:LYS:HE2	2.20	0.56
1:B:87:ASP:HA	1:B:90:LEU:HD11	1.88	0.56
1:B:187:ILE:HD12	1:B:188:GLU:N	2.20	0.56
1:C:410:HIS:N	1:C:411:ALA:HA	2.20	0.56
1:C:358:VAL:HG12	1:C:373:LEU:HD12	1.88	0.56
1:A:108:GLN:NE2	1:C:96:GLN:OE1	2.39	0.56
1:C:206:ASP:HA	1:C:209:LYS:HD2	1.87	0.56
1:B:94:LEU:N	1:B:94:LEU:HD23	2.21	0.55
1:C:174:ASN:ND2	1:C:177:GLU:OE1	2.39	0.55
1:D:358:VAL:HG12	1:D:373:LEU:HD12	1.88	0.55
1:B:94:LEU:HB3	1:B:113:LEU:HD22	1.89	0.55
1:B:358:VAL:HG12	1:B:373:LEU:HD12	1.88	0.55
1:D:382:ASP:O	1:D:427:HIS:CE1	2.60	0.55
1:D:261:PHE:HB2	1:D:294:PHE:CD1	2.43	0.54
1:A:186:GLN:OE1	1:A:191:LYS:HG2	2.08	0.54
1:A:261:PHE:HB2	1:A:294:PHE:CD1	2.43	0.54
1:A:358:VAL:HG12	1:A:373:LEU:HD12	1.88	0.54
1:C:110:GLY:HA3	1:C:152:MET:HE3	1.90	0.53
1:D:438:VAL:HG12	1:D:443:ILE:HD11	1.90	0.53
1:B:186:GLN:OE1	1:B:191:LYS:CD	2.54	0.53
1:D:186:GLN:HE21	1:D:186:GLN:N	2.06	0.53
1:D:514:MET:O	1:D:517:GLU:CA	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:ND2	1:A:328:VAL:HG23	2.24	0.53
1:B:261:PHE:HB2	1:B:294:PHE:CD1	2.43	0.53
1:C:261:PHE:HB2	1:C:294:PHE:CD1	2.44	0.53
1:A:514:MET:CB	1:A:517:GLU:CB	2.87	0.53
1:B:322:GLU:HB2	1:B:323:ASP:HB2	1.91	0.53
1:B:90:LEU:N	1:B:90:LEU:HD13	2.16	0.53
1:D:410:HIS:N	1:D:411:ALA:HA	2.24	0.53
1:A:173:THR:HG23	1:A:175:ILE:HG22	1.91	0.52
1:C:438:VAL:HG12	1:C:443:ILE:HD11	1.91	0.52
1:D:221:LEU:HD21	1:D:246:LEU:HD23	1.92	0.52
1:A:438:VAL:HG12	1:A:443:ILE:HD11	1.92	0.52
1:B:221:LEU:HD21	1:B:246:LEU:HD23	1.92	0.52
1:B:438:VAL:HG12	1:B:443:ILE:HD11	1.91	0.51
1:D:91:ILE:HD11	1:D:123:LEU:HD12	1.91	0.51
1:C:106:LEU:HA	1:C:109:THR:HG22	1.92	0.51
1:A:91:ILE:HD11	1:A:123:LEU:HD23	1.93	0.51
1:A:221:LEU:HD21	1:A:246:LEU:HD23	1.92	0.50
1:A:187:ILE:HD12	1:A:187:ILE:H	1.76	0.50
1:A:106:LEU:HA	1:A:109:THR:HG22	1.94	0.50
1:B:106:LEU:HA	1:B:109:THR:HG22	1.93	0.50
1:C:221:LEU:HD21	1:C:246:LEU:HD23	1.93	0.50
1:B:87:ASP:C	1:B:90:LEU:HD21	2.26	0.50
1:C:325:ASN:OD1	1:C:325:ASN:C	2.51	0.50
1:B:91:ILE:CG2	1:B:130:MET:CE	2.88	0.49
1:D:106:LEU:HA	1:D:109:THR:HG22	1.93	0.49
1:A:173:THR:OG1	1:A:174:ASN:N	2.45	0.49
1:B:497:ARG:HA	1:B:499:ALA:O	2.13	0.49
1:C:173:THR:OG1	1:C:175:ILE:HG22	2.13	0.49
1:C:498:SER:CB	1:C:501:GLU:H	2.25	0.48
1:D:187:ILE:C	1:D:187:ILE:HD12	2.33	0.48
1:C:175:ILE:HG12	1:C:179:LEU:HD22	1.95	0.48
1:B:113:LEU:HA	1:B:116:ILE:HG12	1.96	0.48
1:C:90:LEU:O	1:C:94:LEU:HD23	2.13	0.48
1:D:514:MET:C	1:D:517:GLU:CB	2.79	0.48
1:B:326:VAL:HG21	1:B:366:MET:HG3	1.96	0.48
1:A:326:VAL:HG21	1:A:366:MET:HG3	1.97	0.47
1:B:409:ASP:CB	1:B:410:HIS:HA	2.44	0.47
1:C:326:VAL:HG21	1:C:366:MET:HG3	1.97	0.47
1:B:175:ILE:HG12	1:B:179:LEU:HD22	1.95	0.47
1:A:175:ILE:HG12	1:A:179:LEU:HD22	1.96	0.47
1:C:187:ILE:HD12	1:C:188:GLU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ASN:CG	1:C:327:THR:HG23	2.26	0.47
1:D:514:MET:O	1:D:517:GLU:N	2.48	0.47
1:D:175:ILE:HG12	1:D:179:LEU:HD22	1.96	0.47
1:B:186:GLN:OE1	1:B:191:LYS:CE	2.63	0.46
1:C:409:ASP:CB	1:C:410:HIS:HA	2.42	0.46
1:D:90:LEU:O	1:D:94:LEU:HD23	2.15	0.46
1:C:187:ILE:HD12	1:C:187:ILE:H	1.81	0.46
1:A:187:ILE:HD12	1:A:188:GLU:H	1.81	0.46
1:D:326:VAL:HG21	1:D:366:MET:HG3	1.97	0.46
1:A:130:MET:N	1:A:131:GLY:HA2	2.31	0.46
1:B:499:ALA:C	1:B:502:ILE:H	2.19	0.46
1:B:94:LEU:HA	1:B:97:LEU:HD12	1.98	0.46
1:B:96:GLN:HG2	1:D:108:GLN:NE2	2.31	0.46
1:D:395:VAL:O	1:D:399:GLU:HG3	2.16	0.45
1:C:186:GLN:CD	1:C:191:LYS:HG2	2.35	0.45
1:A:273:LEU:HD23	1:A:276:ILE:HD12	1.99	0.45
1:A:152:MET:HG2	1:A:152:MET:O	2.16	0.45
1:B:130:MET:N	1:B:131:GLY:HA2	2.31	0.45
1:B:187:ILE:HD12	1:B:188:GLU:H	1.81	0.45
1:A:325:ASN:OD1	1:A:327:THR:HG22	2.17	0.45
1:A:395:VAL:O	1:A:399:GLU:HG3	2.16	0.45
1:B:395:VAL:O	1:B:399:GLU:HG3	2.17	0.45
1:B:173:THR:OG1	1:B:175:ILE:HG22	2.16	0.45
1:C:395:VAL:O	1:C:399:GLU:HG3	2.17	0.45
1:D:273:LEU:HD23	1:D:276:ILE:HD12	1.99	0.45
1:B:90:LEU:O	1:B:94:LEU:HD23	2.17	0.45
1:B:381:ILE:O	1:B:381:ILE:CD1	2.58	0.44
1:B:349:MET:O	1:B:354:VAL:HG22	2.18	0.44
1:D:130:MET:N	1:D:131:GLY:HA2	2.33	0.44
1:A:92:SER:HG	1:A:93:PRO:HD3	1.80	0.44
1:B:273:LEU:HD23	1:B:276:ILE:HD12	1.98	0.44
1:C:273:LEU:HD23	1:C:276:ILE:HD12	1.98	0.44
1:D:264:GLY:O	1:D:303:HIS:ND1	2.50	0.44
1:B:499:ALA:O	1:B:502:ILE:CB	2.65	0.44
1:B:501:GLU:O	1:B:504:TYR:N	2.45	0.43
1:A:186:GLN:CD	1:A:191:LYS:HG2	2.38	0.43
1:B:90:LEU:N	1:B:90:LEU:HD22	2.32	0.43
1:C:130:MET:N	1:C:131:GLY:HA2	2.32	0.43
1:D:120:SER:OG	1:D:123:LEU:HD23	2.19	0.43
1:D:90:LEU:O	1:D:93:PRO:HD2	2.19	0.43
1:C:210:LEU:O	1:C:213:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ASN:HB3	1:D:283:LEU:HB2	2.01	0.43
1:B:92:SER:HB2	1:B:93:PRO:CD	2.49	0.43
1:B:317:LEU:HD22	1:B:361:PHE:CE2	2.54	0.43
1:C:187:ILE:HD12	1:C:188:GLU:N	2.33	0.43
1:A:264:GLY:O	1:A:303:HIS:ND1	2.52	0.42
1:A:446:LEU:O	1:A:461:ALA:HB1	2.19	0.42
1:A:90:LEU:O	1:A:93:PRO:HD2	2.20	0.42
1:C:280:ASN:HB3	1:C:283:LEU:HB2	2.00	0.42
1:B:499:ALA:HB3	1:B:500:PRO:CA	2.49	0.42
1:D:196:PHE:CG	1:D:242:THR:HG21	2.54	0.42
1:A:264:GLY:HA2	1:A:265:LYS:HA	1.85	0.42
1:A:409:ASP:CB	1:A:410:HIS:HA	2.43	0.42
1:D:196:PHE:CD2	1:D:242:THR:HG21	2.55	0.42
1:D:317:LEU:HD22	1:D:361:PHE:CE2	2.55	0.42
1:B:196:PHE:CD2	1:B:242:THR:HG21	2.55	0.42
1:B:90:LEU:HD22	1:B:91:ILE:N	2.34	0.42
1:B:96:GLN:HG2	1:D:108:GLN:HE21	1.85	0.42
1:A:280:ASN:HB3	1:A:283:LEU:HB2	2.02	0.42
1:A:317:LEU:HD22	1:A:361:PHE:CE2	2.55	0.42
1:C:325:ASN:OD1	1:C:328:VAL:N	2.49	0.42
1:C:118:TYR:HA	1:C:119:ASP:HA	1.87	0.41
1:C:90:LEU:O	1:C:93:PRO:HD2	2.20	0.41
1:B:446:LEU:O	1:B:461:ALA:HB1	2.20	0.41
1:B:499:ALA:HB3	1:B:500:PRO:C	2.40	0.41
1:C:105:VAL:O	1:C:109:THR:HG22	2.21	0.41
1:C:446:LEU:O	1:C:461:ALA:HB1	2.20	0.41
1:D:105:VAL:O	1:D:109:THR:HG22	2.20	0.41
1:D:382:ASP:O	1:D:427:HIS:ND1	2.53	0.41
1:C:196:PHE:CD2	1:C:242:THR:HG21	2.56	0.41
1:C:196:PHE:CG	1:C:242:THR:HG21	2.55	0.41
1:A:196:PHE:CG	1:A:242:THR:HG21	2.55	0.41
1:D:409:ASP:CB	1:D:410:HIS:HA	2.45	0.41
1:A:105:VAL:O	1:A:109:THR:HG22	2.21	0.41
1:B:105:VAL:O	1:B:109:THR:HG22	2.20	0.41
1:C:151:GLU:O	1:C:155:VAL:HG23	2.21	0.41
1:D:446:LEU:O	1:D:461:ALA:HB1	2.21	0.41
1:B:187:ILE:CD1	1:B:188:GLU:N	2.84	0.41
1:B:90:LEU:CD2	1:B:91:ILE:N	2.84	0.41
1:C:358:VAL:CG1	1:C:373:LEU:HD12	2.51	0.41
1:A:187:ILE:HD12	1:A:188:GLU:N	2.36	0.41
1:A:358:VAL:CG1	1:A:373:LEU:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:PHE:CG	1:B:242:THR:HG21	2.55	0.41
1:C:499:ALA:O	1:C:502:ILE:N	2.53	0.41
1:C:264:GLY:O	1:C:303:HIS:ND1	2.53	0.41
1:B:280:ASN:HB3	1:B:283:LEU:HB2	2.02	0.40
1:D:411:ALA:HB1	1:D:414:MET:HB3	2.03	0.40
1:D:438:VAL:CG1	1:D:443:ILE:HD11	2.51	0.40
1:B:264:GLY:O	1:B:303:HIS:ND1	2.55	0.40
1:B:499:ALA:HB1	1:B:502:ILE:N	2.36	0.40
1:B:94:LEU:N	1:B:94:LEU:CD2	2.84	0.40
1:D:323:ASP:HA	1:D:324:GLY:HA3	1.87	0.40
1:D:358:VAL:CG1	1:D:373:LEU:HD12	2.51	0.40
1:D:515:GLY:C	1:D:517:GLU:N	2.75	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	467/487 (96%)	437 (94%)	28 (6%)	2 (0%)	34 72
1	B	467/487 (96%)	438 (94%)	27 (6%)	2 (0%)	34 72
1	C	467/487 (96%)	436 (93%)	29 (6%)	2 (0%)	34 72
1	D	467/487 (96%)	437 (94%)	28 (6%)	2 (0%)	34 72
2	e	155/198 (78%)	146 (94%)	9 (6%)	0	100 100
2	f	150/198 (76%)	140 (93%)	10 (7%)	0	100 100
2	g	150/198 (76%)	139 (93%)	11 (7%)	0	100 100
2	h	155/198 (78%)	146 (94%)	9 (6%)	0	100 100
All	All	2478/2740 (90%)	2319 (94%)	151 (6%)	8 (0%)	41 75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	B	505	ASN
1	D	394	ASN
1	C	394	ASN
1	C	499	ALA
1	D	499	ALA
1	A	324	GLY
1	B	523	VAL

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	340/414 (82%)	304 (89%)	36 (11%)	6 30
1	B	340/414 (82%)	302 (89%)	38 (11%)	6 27
1	C	340/414 (82%)	306 (90%)	34 (10%)	7 32
1	D	340/414 (82%)	305 (90%)	35 (10%)	7 32
2	e	142/169 (84%)	112 (79%)	30 (21%)	1 5
2	f	130/169 (77%)	111 (85%)	19 (15%)	3 18
2	g	130/169 (77%)	112 (86%)	18 (14%)	3 20
2	h	142/169 (84%)	114 (80%)	28 (20%)	1 7
All	All	1904/2332 (82%)	1666 (88%)	238 (12%)	4 23

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	98	LEU
1	A	103	GLN
1	A	107	LEU
1	A	111	ARG
1	A	113	LEU
1	A	115	ASN
1	A	116	ILE

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Mol	Chain	Res	Type
1	A	135	THR
1	A	149	LEU
1	A	152	MET
1	A	153	CYS
1	A	154	LEU
1	A	160	LEU
1	A	173	THR
1	A	179	LEU
1	A	187	ILE
1	A	199	LEU
1	A	227	GLN
1	A	271	ARG
1	A	273	LEU
1	A	311	GLU
1	A	326	VAL
1	A	355	THR
1	A	373	LEU
1	A	393	LYS
1	A	397	LEU
1	A	418	ASN
1	A	421	LEU
1	A	455	VAL
1	A	456	ILE
1	A	465	LEU
1	A	467	LEU
1	A	468	ILE
1	A	487	GLN
1	A	491	ARG
1	B	90	LEU
1	B	92	SER
1	B	94	LEU
1	B	96	GLN
1	B	98	LEU
1	B	103	GLN
1	B	107	LEU
1	B	111	ARG
1	B	113	LEU
1	B	135	THR
1	B	149	LEU
1	B	153	CYS
1	B	154	LEU
1	B	160	LEU

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Mol	Chain	Res	Type
1	B	169	GLN
1	B	179	LEU
1	B	187	ILE
1	B	199	LEU
1	B	227	GLN
1	B	271	ARG
1	B	273	LEU
1	B	311	GLU
1	B	326	VAL
1	B	366	MET
1	B	373	LEU
1	B	381	ILE
1	B	382	ASP
1	B	393	LYS
1	B	397	LEU
1	B	418	ASN
1	B	421	LEU
1	B	455	VAL
1	B	456	ILE
1	B	465	LEU
1	B	467	LEU
1	B	468	ILE
1	B	491	ARG
1	B	492	LEU
1	C	90	LEU
1	C	98	LEU
1	C	107	LEU
1	C	111	ARG
1	C	115	ASN
1	C	116	ILE
1	C	135	THR
1	C	149	LEU
1	C	153	CYS
1	C	154	LEU
1	C	160	LEU
1	C	174	ASN
1	C	179	LEU
1	C	186	GLN
1	C	187	ILE
1	C	199	LEU
1	C	227	GLN
1	C	271	ARG

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Mol	Chain	Res	Type
1	C	273	LEU
1	C	280	ASN
1	C	311	GLU
1	C	322	GLU
1	C	326	VAL
1	C	373	LEU
1	C	393	LYS
1	C	397	LEU
1	C	418	ASN
1	C	421	LEU
1	C	455	VAL
1	C	456	ILE
1	C	465	LEU
1	C	467	LEU
1	C	468	ILE
1	C	491	ARG
1	D	98	LEU
1	D	103	GLN
1	D	107	LEU
1	D	111	ARG
1	D	113	LEU
1	D	116	ILE
1	D	135	THR
1	D	149	LEU
1	D	153	CYS
1	D	154	LEU
1	D	160	LEU
1	D	169	GLN
1	D	174	ASN
1	D	179	LEU
1	D	186	GLN
1	D	187	ILE
1	D	199	LEU
1	D	227	GLN
1	D	271	ARG
1	D	273	LEU
1	D	311	GLU
1	D	322	GLU
1	D	323	ASP
1	D	366	MET
1	D	373	LEU
1	D	393	LYS

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Mol	Chain	Res	Type
1	D	397	LEU
1	D	410	HIS
1	D	421	LEU
1	D	455	VAL
1	D	456	ILE
1	D	465	LEU
1	D	467	LEU
1	D	468	ILE
1	D	491	ARG
2	e	5	ARG
2	e	10	ILE
2	e	11	VAL
2	e	20	CYS
2	e	22	LEU
2	e	25	PHE
2	e	40	GLU
2	e	41	ASN
2	e	43	VAL
2	e	48	VAL
2	e	51	LYS
2	e	52	GLN
2	e	57	LEU
2	e	58	TRP
2	e	65	ASP
2	e	72	LEU
2	e	80	ILE
2	e	85	SER
2	e	90	ASP
2	e	92	LEU
2	e	93	GLU
2	e	104	LYS
2	e	119	LYS
2	e	121	LEU
2	e	140	LYS
2	e	145	ARG
2	e	157	MET
2	e	162	LYS
2	e	172	GLU
2	e	179	LEU
2	f	43	VAL
2	f	45	ASP
2	f	48	VAL

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Mol	Chain	Res	Type
2	f	49	ASP
2	f	51	LYS
2	f	52	GLN
2	f	57	LEU
2	f	58	TRP
2	f	65	ASP
2	f	80	ILE
2	f	85	SER
2	f	104	LYS
2	f	121	LEU
2	f	140	LYS
2	f	145	ARG
2	f	157	MET
2	f	162	LYS
2	f	172	GLU
2	f	180	GLN
2	g	41	ASN
2	g	45	ASP
2	g	48	VAL
2	g	49	ASP
2	g	51	LYS
2	g	52	GLN
2	g	58	TRP
2	g	65	ASP
2	g	80	ILE
2	g	85	SER
2	g	90	ASP
2	g	104	LYS
2	g	121	LEU
2	g	129	ARG
2	g	140	LYS
2	g	145	ARG
2	g	162	LYS
2	g	172	GLU
2	h	5	ARG
2	h	10	ILE
2	h	11	VAL
2	h	18	LYS
2	h	20	CYS
2	h	22	LEU
2	h	42	TYR
2	h	43	VAL

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Mol	Chain	Res	Type
2	h	48	VAL
2	h	49	ASP
2	h	51	LYS
2	h	52	GLN
2	h	57	LEU
2	h	58	TRP
2	h	65	ASP
2	h	80	ILE
2	h	85	SER
2	h	90	ASP
2	h	104	LYS
2	h	121	LEU
2	h	140	LYS
2	h	145	ARG
2	h	162	LYS
2	h	172	GLU
2	h	179	LEU
2	h	180	GLN
2	h	190	CYS
2	h	191	LEU

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

Mol	Chain	Res	Type
1	A	126	GLN
1	A	143	HIS
1	A	258	GLN
1	B	143	HIS
1	B	345	ASN
1	B	384	GLN
1	B	410	HIS
1	B	427	HIS
1	C	103	GLN
1	C	126	GLN
1	C	143	HIS
1	C	159	ASN
1	D	143	HIS
1	D	186	GLN
2	h	117	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands 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	$\#\|Z\| > 2$
3	FAR	g	201	2	14,14,14	2.62	2 (14%)	16,16,16	1.04	1 (6%)
3	FAR	f	201	2	14,14,14	2.60	2 (14%)	16,16,16	1.25	1 (6%)
3	FAR	h	201	2	14,14,14	2.51	2 (14%)	16,16,16	1.17	1 (6%)
3	FAR	e	201	2	14,14,14	2.55	2 (14%)	16,16,16	1.16	2 (12%)

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	FAR	g	201	2	-	5/14/14/14	-
3	FAR	f	201	2	-	5/14/14/14	-
3	FAR	h	201	2	-	6/14/14/14	-
3	FAR	e	201	2	-	6/14/14/14	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	201	FAR	C15-C13	-6.87	1.31	1.50
3	e	201	FAR	C10-C8	-6.74	1.33	1.50
3	f	201	FAR	C10-C8	-6.69	1.33	1.50
3	g	201	FAR	C10-C8	-6.67	1.33	1.50
3	f	201	FAR	C15-C13	-6.61	1.32	1.50
3	h	201	FAR	C10-C8	-6.49	1.34	1.50
3	e	201	FAR	C15-C13	-6.37	1.33	1.50
3	h	201	FAR	C15-C13	-6.36	1.33	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	e	201	FAR	C1-C2-C3	-2.61	120.58	126.57
3	h	201	FAR	C10-C8-C9	2.20	118.97	115.27
3	f	201	FAR	C10-C8-C9	2.09	118.78	115.27
3	e	201	FAR	C10-C8-C9	2.07	118.76	115.27
3	g	201	FAR	C10-C8-C9	2.04	118.70	115.27

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	g	201	FAR	C3-C5-C6-C7
3	f	201	FAR	C3-C5-C6-C7
3	f	201	FAR	C9-C11-C12-C13
3	h	201	FAR	C12-C11-C9-C8
3	e	201	FAR	C12-C11-C9-C8
3	h	201	FAR	C10-C8-C9-C11
3	e	201	FAR	C10-C8-C9-C11
3	f	201	FAR	C4-C3-C5-C6
3	f	201	FAR	C2-C3-C5-C6
3	h	201	FAR	C7-C8-C9-C11
3	g	201	FAR	C4-C3-C5-C6
3	e	201	FAR	C7-C8-C9-C11
3	g	201	FAR	C2-C3-C5-C6
3	h	201	FAR	C4-C3-C5-C6
3	e	201	FAR	C4-C3-C5-C6
3	h	201	FAR	C3-C5-C6-C7
3	h	201	FAR	C2-C3-C5-C6
3	e	201	FAR	C2-C3-C5-C6
3	g	201	FAR	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	g	201	FAR	C5-C6-C7-C8
3	e	201	FAR	C3-C5-C6-C7
3	f	201	FAR	C5-C6-C7-C8

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	469/487 (96%)	-0.50	2 (0%) 92 90	79, 124, 170, 232	0
1	B	469/487 (96%)	-0.29	7 (1%) 73 68	66, 136, 219, 273	0
1	C	469/487 (96%)	-0.46	2 (0%) 92 90	73, 119, 165, 199	0
1	D	469/487 (96%)	-0.59	1 (0%) 95 93	64, 106, 151, 195	0
2	e	163/198 (82%)	0.45	18 (11%) 5 6	86, 179, 263, 305	0
2	f	156/198 (78%)	0.06	6 (3%) 40 36	93, 162, 213, 242	0
2	g	156/198 (78%)	-0.17	2 (1%) 77 71	72, 130, 204, 256	0
2	h	163/198 (82%)	-0.05	6 (3%) 41 37	73, 154, 213, 318	0
All	All	2514/2740 (91%)	-0.32	44 (1%) 68 62	64, 126, 211, 318	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	h	50	GLY	10.2
2	e	49	ASP	8.9
2	h	49	ASP	6.6
2	e	122	ARG	5.1
1	A	555	THR	4.9
2	e	133	LYS	4.2
2	e	83	CYS	4.1
1	B	498	SER	4.0
1	A	118	TYR	3.9
2	e	134	MET	3.9
2	e	129	ARG	3.8
2	e	127	THR	3.8
2	e	50	GLY	3.7
2	e	85	SER	3.7
1	D	555	THR	3.5
2	e	48	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	e	27	LYS	3.0
2	e	138	PRO	2.8
2	h	129	ARG	2.8
2	e	125	GLU	2.7
2	e	132	ALA	2.6
1	B	525	ASP	2.6
2	e	161	ALA	2.6
1	B	471	LEU	2.5
1	C	555	THR	2.4
1	B	555	THR	2.4
2	f	122	ARG	2.4
2	f	120	ASP	2.4
2	e	158	GLU	2.4
1	C	453	GLU	2.3
2	h	127	THR	2.3
1	B	88	ALA	2.3
2	f	134	MET	2.2
2	f	49	ASP	2.2
2	g	46	ILE	2.2
2	h	27	LYS	2.1
2	g	47	GLU	2.1
2	e	160	SER	2.1
2	f	52	GLN	2.1
2	f	163	THR	2.1
2	e	116	GLY	2.1
2	h	121	LEU	2.0
1	B	542	SER	2.0
1	B	554	LEU	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 carbohydrates 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	FAR	e	201	15/15	0.84	0.29	117,126,149,153	0
3	FAR	g	201	15/15	0.85	0.27	112,120,149,150	0
3	FAR	h	201	15/15	0.92	0.20	84,96,128,139	0
3	FAR	f	201	15/15	0.95	0.23	79,85,100,102	0

6.5 Other polymers (i)

There are no such residues in this entry.