WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 01:40 PM EDT

PDB ID : 4RRP

Title : Crystal Structure of the Fab complexed with antigen Asf1p, Northeast Structural Genomics Consortium (NESG) Target PdR16

Authors : Kuzin, A.; Lew, S.; Seetharaman, J.; Mao, L.; Xiao, R.; Oconnell, P.T.; Maglaqui, M.; Bailey, L.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Chaperone-Enabled Studies of Epigenetic Regulation Enzymes (CEBS); Northeast Structural Genomics Consortium (NESG)

Deposited on : 2014-11-06

Resolution : 2.79 Å(reported)

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

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

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 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
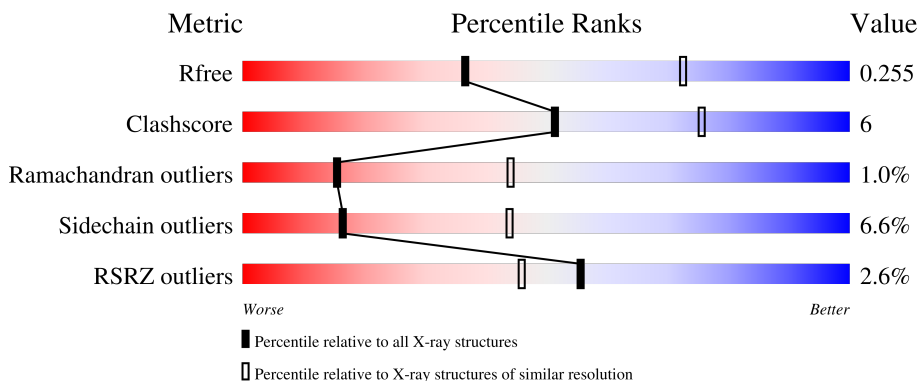
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	83% 14% ••
1	B	216	85% 14%
1	C	216	% 73% 22% • •
1	D	216	85% 14% •

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Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
1	E	216	79% 20%
1	F	216	7% 68% 28%
2	G	238	77% 13% 8%
2	H	238	79% 13% 7%
2	I	238	3% 74% 16% 8%
2	J	238	85% 7% 7%
2	K	238	3% 66% 21% 10%
2	L	238	13% 67% 21% 10%
3	M	160	% 80% 15%
3	N	160	3% 76% 18% 5%
3	O	160	% 86% 9%
3	P	160	% 83% 13%
3	Q	160	3% 72% 22%
3	R	160	6% 71% 18% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27161 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 Fab antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total 1655	C 1035	N 282	O 333	S 5	0	2	0
1	B	216	Total 1656	C 1035	N 278	O 336	S 7	0	0	0
1	C	212	Total 1627	C 1019	N 274	O 329	S 5	0	0	0
1	D	214	Total 1650	C 1032	N 279	O 333	S 6	0	1	0
1	E	214	Total 1642	C 1027	N 276	O 334	S 5	0	0	0
1	F	214	Total 1642	C 1027	N 276	O 333	S 6	0	0	0

- Molecule 2 is a protein called Fab antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	219	Total 1633	C 1031	N 272	O 323	S 7	0	1	0
2	H	221	Total 1651	C 1041	N 276	O 328	S 6	0	1	0
2	I	220	Total 1634	C 1032	N 271	O 325	S 6	0	0	0
2	J	222	Total 1646	C 1038	N 273	O 328	S 7	0	0	0
2	K	214	Total 1598	C 1012	N 264	O 316	S 6	0	0	0
2	L	214	Total 1599	C 1012	N 264	O 316	S 7	0	0	0

- Molecule 3 is a protein called Antigen Asf1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	153	Total 1222	C 784	N 198	O 238	S 2	0	0	0
3	N	152	Total 1225	C 788	N 199	O 236	S 2	0	1	0
3	O	153	Total 1218	C 781	N 196	O 239	S 2	0	0	0
3	P	156	Total 1252	C 802	N 206	O 242	S 2	0	1	0
3	Q	153	Total 1234	C 794	N 201	O 237	S 2	0	1	0
3	R	143	Total 1147	C 737	N 187	O 221	S 2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	GLY	-	expression tag	UNP E7KE71
M	1	SER	-	expression tag	UNP E7KE71
N	0	GLY	-	expression tag	UNP E7KE71
N	1	SER	-	expression tag	UNP E7KE71
O	0	GLY	-	expression tag	UNP E7KE71
O	1	SER	-	expression tag	UNP E7KE71
P	0	GLY	-	expression tag	UNP E7KE71
P	1	SER	-	expression tag	UNP E7KE71
Q	0	GLY	-	expression tag	UNP E7KE71
Q	1	SER	-	expression tag	UNP E7KE71
R	0	GLY	-	expression tag	UNP E7KE71
R	1	SER	-	expression tag	UNP E7KE71

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 4	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total 21	O 21	0	0
5	G	22	Total 22	O 22	0	0
5	B	20	Total 20	O 20	0	0
5	H	27	Total 27	O 27	0	0
5	C	15	Total 15	O 15	0	0
5	I	14	Total 14	O 14	0	0
5	D	16	Total 16	O 16	0	0
5	J	21	Total 21	O 21	0	0
5	K	3	Total 3	O 3	0	0
5	F	3	Total 3	O 3	0	0
5	L	2	Total 2	O 2	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	10	Total 10	O 10	0	0
5	N	15	Total 15	O 15	0	0
5	O	16	Total 16	O 16	0	0
5	P	13	Total 13	O 13	0	0
5	Q	3	Total 3	O 3	0	0
5	R	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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.
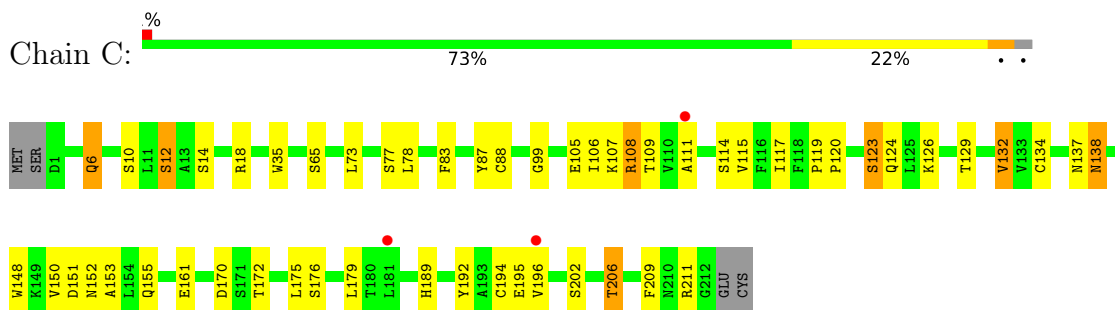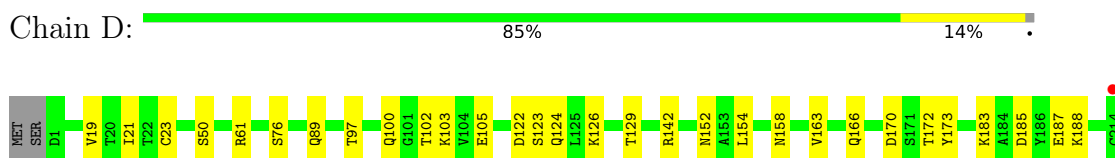
• Molecule 1: Fab antibody, light chain
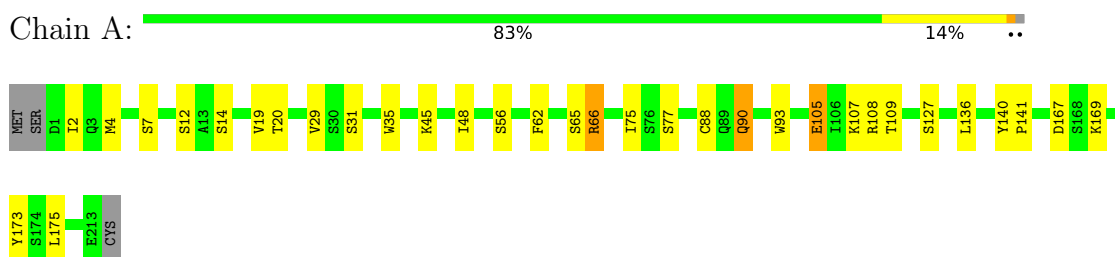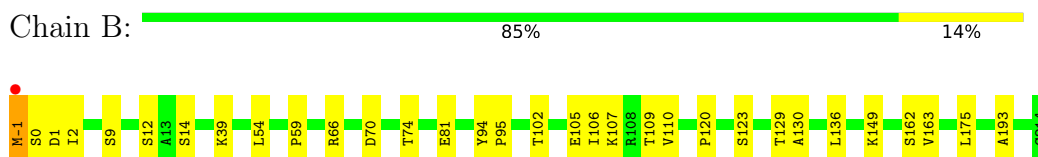
Chain A:

• Molecule 1: Fab antibody, light chain
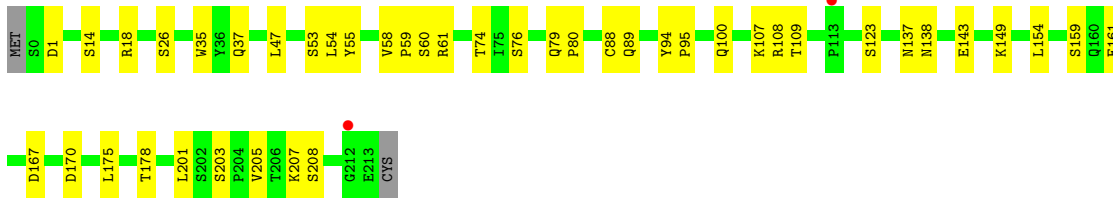
Chain B:

• Molecule 1: Fab antibody, light chain

Chain C:
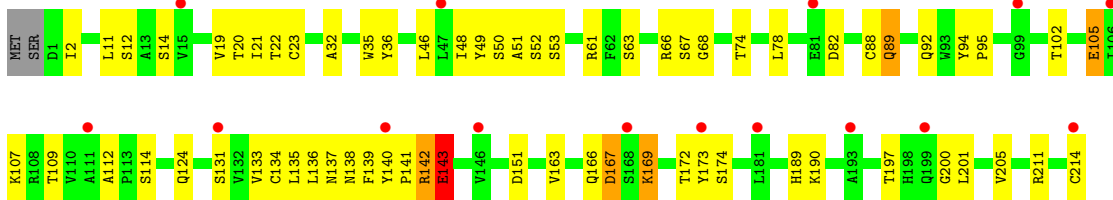
• Molecule 1: Fab antibody, light chain

Chain D:

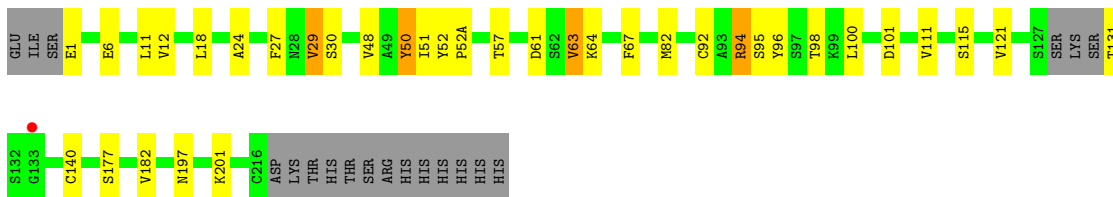• Molecule 1: Fab antibody, light chain

Chain E:

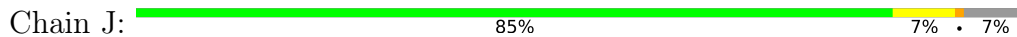• Molecule 1: Fab antibody, light chain

Chain F:

• Molecule 2: Fab antibody, heavy chain

Chain G:

• Molecule 2: Fab antibody, heavy chain

Chain H:

• Molecule 2: Fab antibody, heavy chain

Chain I:

W154 L159 Q171 S177 V182 T183 V184 P185 S186 S187 S188 L189 G190 T191 Q192 T193 Y194 K210 V211 E212 P213 K214 SER CYS ASP LYS THR HIS THR SER ARG HIS HIS HIS HIS HIS HIS

• Molecule 2: Fab antibody, heavy chain

Chain J:

GLU ILE SER E1 E6 S21 D61 S62 V63 F67 A93 R94 M100B S115 W154 S161 A168 L178 T191 Q192 C196 N197 V198 N199 H200 K201 N204 C216 ASP LYS THR HIS THR SER ARG HIS HIS HIS HIS HIS HIS

• Molecule 2: Fab antibody, heavy chain

Chain K:

GLU ILE SER E1 V5 E6 L11 L18 A23 A24 V29 S32 S33 I34 H35 R38 I51 Y52 P52A S58 D61 S62 V63 R66 F67 T68 N76 M82 N82A S82B L82C E85 D86 T87 Y90 A93 R94 S95 M100B D101 T110

P119 P126 K129 SER THR SER GLY GLY T135 L138 D144 E148 P149 V150 T151 W154 L159 A168 Q171 S172 S173 L178 V182 T183 V184 P185 T191 Q192 T193 Y194 N199 H200 K201 P202 S203 N204 T205 K206 V207 D208 P213 LYS SER CYS LYS

THR HIS THR SER ARG HIS HIS HIS HIS HIS HIS

• Molecule 2: Fab antibody, heavy chain

Chain L:

GLU ILE SER E1 A23 A24 F27 N28 V29 H35 Q39 A40 P41 L45 E46 W47 Y50 I51 Y52 P52A S58 V63 F67 N76 R83 A84 E85 A88 V89 C92 A93 R94 S95 Y96 K99 L100 A100A M100B D101 Y102 W103 G104 Q105 L108

S112 S115 T116 K117 G118 P119 S120 V121 S127 S128 LYS SER THR SER GLY GLY T135 L138 G139 C140 L141 V142 K143 D144 Y145 P146 P147 E148 P149 V150 T151 W154 A158 L159 T160 S161 T165 F166 V169 S172 S173 G174 L175 Y176 S177 L178 V181 V184 P185 S186

L189 GLY THR Q192 H200 K201 P202 T205 K206 V207 D208 V211 S215 C216 ASP LYS THR HIS THR SER ARG HIS HIS HIS HIS HIS HIS

• Molecule 3: Antigen Asf1p

Chain M:

G0 S5 I9 L12 T19 E29 D37 V45 G46 S47 SER ARG SER LEU ASP H53 D54 Q55 G63 V67 G68 V69 P78 L89 V90 L96 L97 D118 E121 L122 R123 E124 V130 E156 N157 GLU GLY

• Molecule 3: Antigen Asf1p

Chain N:

GLY S1 K10 N13 L42 S47 SER ARG SER L51 D52 H53 D54 Q55 E56 S59 I60 L61 V62 G63 P64 V69 S80 L83 L89 I95 L96 L97 F106 N114 N115 E116 Y117 E120 R123 E124 N125 V132 I139 L140 A141 E142 K143 P144

R145 I151 V152 W153 D154 N155 GLU ASN GLY

• Molecule 3: Antigen Asf1p

Chain O:

%

86%   9% •

G0 S1 S2 I9 T19 S48 ARG SER LEU ASP HIS D54 L61 L89 L97 F106 V109 E124 V130 Q131 V132 K143 V146 F149 N157 GLU GLY

• Molecule 3: Antigen Asf1p

Chain P:

%

83%   13% • •

G0 L6 F18 W40 T43 R49 S50 L51 D52 H53 D58 S59 S80 L83 I95 Y111 E120 R123 V132 I135 I139 L140 A141 P144 R145 R148 V152 N155 GLU ASN GLU GLY

• Molecule 3: Antigen Asf1p

Chain Q:

3%

72%   22% • •

GLY SER SER I3 V4 S5 V11 T19 F24 T27 F28 E29 C30 L31 L34 K35 H36 D37 W40 Y44 L51 L57 D58 S59 G63 V67 P78 E82 S91 I95 L96 C99 S100 Y101 F106 V107 Y111 Y112 Y113 I139 L140

K143 P144 F149 W153 D154 N155 GLU ASN GLY

• Molecule 3: Antigen Asf1p

Chain R:

6%

71%   18% •   11%

GLY S1 S2 I3 L12 L31 E32 S33 L34 W40 K41 L42 T43 Y44 S48 ARG SER LEU ASP H53 D54 Q55 E56 L57 D58 S59 I60 F74 S80 A81 GLU LEU ILE PRO ALA SER GLU LEU V90 V94 I95 C99 Y111 Y112 Y113 Y117 D118 E119 E120 E121

E124 N125 P126 P127 A128 K129 V130 Q131 V132 D133 E142 K143 P144 V152 N155 GLU ASN GLU GLY

4 Data and refinement statistics ⓘ

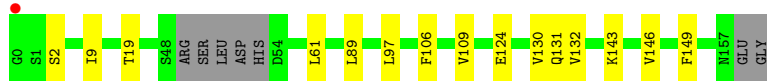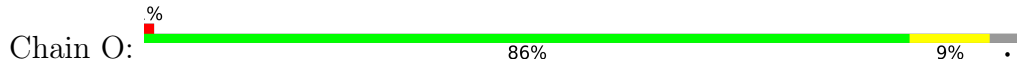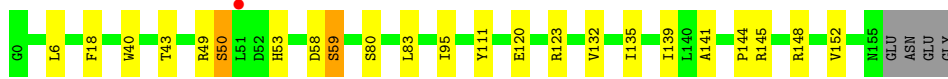| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.72Å 181.31Å 259.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.79 49.69 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.69-2.79) 99.4 (49.69-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.253 0.186 , 0.255	Depositor DCC
R_{free} test set	1999 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27161	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PEG

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	0.50	0/1694	0.60	0/2299
1	B	0.52	0/1692	0.60	1/2297 (0.0%)
1	C	0.49	0/1663	0.59	0/2259
1	D	0.52	0/1689	0.61	0/2293
1	E	0.41	0/1678	0.53	0/2279
1	F	0.37	0/1678	0.55	0/2279
2	G	0.53	0/1675	0.63	0/2283
2	H	0.51	0/1691	0.60	1/2305 (0.0%)
2	I	0.51	0/1674	0.67	2/2283 (0.1%)
2	J	0.53	0/1686	0.64	0/2299
2	K	0.38	0/1637	0.51	0/2233
2	L	0.38	0/1637	0.54	0/2231
3	M	0.50	0/1250	0.60	0/1704
3	N	0.47	0/1256	0.61	0/1712
3	O	0.51	0/1245	0.60	0/1697
3	P	0.52	0/1284	0.59	0/1750
3	Q	0.40	0/1266	0.55	0/1727
3	R	0.40	0/1173	0.55	0/1597
All	All	0.47	0/27568	0.59	4/37527 (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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	138	LEU	CA-CB-CG	5.95	128.97	115.30
2	I	66	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	66	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	H	178	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	-1	MET	Peptide

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	1655	0	1619	18	0
1	B	1656	0	1613	17	0
1	C	1627	0	1588	25	0
1	D	1650	0	1612	12	0
1	E	1642	0	1599	17	0
1	F	1642	0	1599	37	0
2	G	1633	0	1601	16	0
2	H	1651	0	1619	15	0
2	I	1634	0	1602	20	0
2	J	1646	0	1612	8	0
2	K	1598	0	1565	36	0
2	L	1599	0	1564	27	0
3	M	1222	0	1197	12	0
3	N	1225	0	1210	13	0
3	O	1218	0	1195	5	0
3	P	1252	0	1237	11	0
3	Q	1234	0	1221	16	0
3	R	1147	0	1124	12	0
4	A	7	0	10	3	0
5	A	21	0	0	0	0
5	B	20	0	0	0	0
5	C	15	0	0	0	0
5	D	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	3	0	0	0	0
5	G	22	0	0	1	0
5	H	27	0	0	0	0
5	I	14	0	0	0	0
5	J	21	0	0	0	0
5	K	3	0	0	0	0
5	L	2	0	0	0	0
5	M	10	0	0	0	0
5	N	15	0	0	0	0
5	O	16	0	0	0	0
5	P	13	0	0	0	0
5	Q	3	0	0	0	0
5	R	2	0	0	0	0
All	All	27161	0	26387	301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 301 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:189:HIS:O	1:C:211:ARG:NH1	2.12	0.81
3:Q:35:LYS:O	3:Q:36:HIS:ND1	2.17	0.76
1:F:214:CYS:HG	2:L:127:SER:HG	1.34	0.75
1:C:120:PRO:HD3	1:C:132:VAL:HG13	1.70	0.73
1:F:12:SER:HB2	1:F:107:LYS:HD3	1.70	0.73

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	213/216 (99%)	201 (94%)	10 (5%)	2 (1%)	17	46
1	B	214/216 (99%)	201 (94%)	12 (6%)	1 (0%)	29	61
1	C	210/216 (97%)	197 (94%)	12 (6%)	1 (0%)	29	61
1	D	213/216 (99%)	198 (93%)	15 (7%)	0	100	100
1	E	212/216 (98%)	189 (89%)	22 (10%)	1 (0%)	29	61
1	F	212/216 (98%)	182 (86%)	27 (13%)	3 (1%)	11	34
2	G	216/238 (91%)	212 (98%)	3 (1%)	1 (0%)	29	61
2	H	220/238 (92%)	213 (97%)	7 (3%)	0	100	100
2	I	218/238 (92%)	203 (93%)	14 (6%)	1 (0%)	29	61
2	J	220/238 (92%)	212 (96%)	8 (4%)	0	100	100
2	K	210/238 (88%)	189 (90%)	18 (9%)	3 (1%)	11	34
2	L	208/238 (87%)	184 (88%)	18 (9%)	6 (3%)	4	15
3	M	149/160 (93%)	142 (95%)	3 (2%)	4 (3%)	5	17
3	N	149/160 (93%)	139 (93%)	8 (5%)	2 (1%)	12	36
3	O	149/160 (93%)	142 (95%)	5 (3%)	2 (1%)	12	36
3	P	155/160 (97%)	146 (94%)	8 (5%)	1 (1%)	25	56
3	Q	152/160 (95%)	137 (90%)	14 (9%)	1 (1%)	22	53
3	R	137/160 (86%)	121 (88%)	12 (9%)	4 (3%)	4	15
All	All	3457/3684 (94%)	3208 (93%)	216 (6%)	33 (1%)	15	44

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	172	SER
1	F	138	ASN
2	L	207	VAL
3	O	130	VAL
3	R	3	ILE

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	190/191 (100%)	180 (95%)	10 (5%)	22	54
1	B	191/191 (100%)	183 (96%)	8 (4%)	30	63
1	C	187/191 (98%)	168 (90%)	19 (10%)	7	22
1	D	190/191 (100%)	181 (95%)	9 (5%)	26	59
1	E	189/191 (99%)	175 (93%)	14 (7%)	13	37
1	F	189/191 (99%)	171 (90%)	18 (10%)	8	25
2	G	183/201 (91%)	168 (92%)	15 (8%)	11	33
2	H	185/201 (92%)	172 (93%)	13 (7%)	15	40
2	I	183/201 (91%)	171 (93%)	12 (7%)	16	44
2	J	185/201 (92%)	176 (95%)	9 (5%)	25	57
2	K	179/201 (89%)	164 (92%)	15 (8%)	11	31
2	L	180/201 (90%)	167 (93%)	13 (7%)	14	38
3	M	140/146 (96%)	135 (96%)	5 (4%)	35	69
3	N	141/146 (97%)	131 (93%)	10 (7%)	14	39
3	O	140/146 (96%)	135 (96%)	5 (4%)	35	69
3	P	144/146 (99%)	136 (94%)	8 (6%)	21	51
3	Q	142/146 (97%)	130 (92%)	12 (8%)	10	31
3	R	132/146 (90%)	123 (93%)	9 (7%)	16	42
All	All	3070/3228 (95%)	2866 (93%)	204 (7%)	16	44

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	68	THR
2	L	58	SER
3	R	80	SER
2	K	110	THR
1	F	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	164	HIS
2	I	199	ASN
1	F	89	GLN
2	H	28	ASN

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Mol	Chain	Res	Type
1	B	137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\#\|Z\| > 2$
4	PEG	A	701	-	6,6,6	0.50	0	5,5,5	0.87	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
4	PEG	A	701	-	-	0/4/4/4	-

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	PEG	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	213/216 (98%)	-0.23	0	100	100	13, 26, 42, 61	0
1	B	216/216 (100%)	-0.31	1 (0%)	91	88	15, 33, 53, 76	0
1	C	212/216 (98%)	0.03	3 (1%)	75	70	12, 41, 71, 80	0
1	D	214/216 (99%)	-0.24	1 (0%)	91	88	14, 25, 43, 74	0
1	E	214/216 (99%)	0.02	2 (0%)	84	80	32, 52, 68, 83	0
1	F	214/216 (99%)	0.67	15 (7%)	16	9	50, 71, 86, 104	0
2	G	219/238 (92%)	-0.34	1 (0%)	91	88	14, 23, 47, 74	0
2	H	221/238 (92%)	-0.22	1 (0%)	91	88	15, 26, 59, 86	0
2	I	220/238 (92%)	0.01	8 (3%)	42	32	12, 28, 75, 89	0
2	J	222/238 (93%)	-0.45	0	100	100	11, 25, 45, 70	0
2	K	214/238 (89%)	0.22	6 (2%)	53	43	26, 63, 87, 106	0
2	L	214/238 (89%)	0.79	30 (14%)	2	1	31, 68, 96, 104	0
3	M	153/160 (95%)	-0.09	1 (0%)	87	84	16, 29, 64, 81	0
3	N	152/160 (95%)	0.05	5 (3%)	46	36	17, 34, 79, 88	1 (0%)
3	O	153/160 (95%)	-0.16	1 (0%)	87	84	15, 27, 68, 79	0
3	P	156/160 (97%)	-0.26	1 (0%)	89	86	16, 25, 54, 76	0
3	Q	153/160 (95%)	0.27	5 (3%)	46	36	28, 54, 86, 95	0
3	R	143/160 (89%)	0.52	9 (6%)	20	12	32, 64, 96, 106	0
All	All	3503/3684 (95%)	0.01	90 (2%)	56	46	11, 36, 82, 106	1 (0%)

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	112	SER	5.7
2	L	119	PRO	4.7
2	L	149	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	L	161	SER	4.2
1	F	106	ILE	4.1

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	PEG	A	701	7/7	0.95	0.31	31,37,43,43	0

6.5   Other polymers ⓘ

There are no such residues in this entry.