Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 PM GMT

PDB ID	:	4M17
Title	:	Crystal Structure of Surfactant Protein-D D325A/R343V mutant
Authors	:	Goh, B.C.; Rynkiewicz, M.J.; Cafarella, T.R.; White, M.R.; Hartshorn, K.L.; Allen, K.; Crouch, E.C.; Calin, O.; Seeberger, P.H.; Schulten, K.; Seaton, B.A.
Deposited on	:	2013-08-02
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

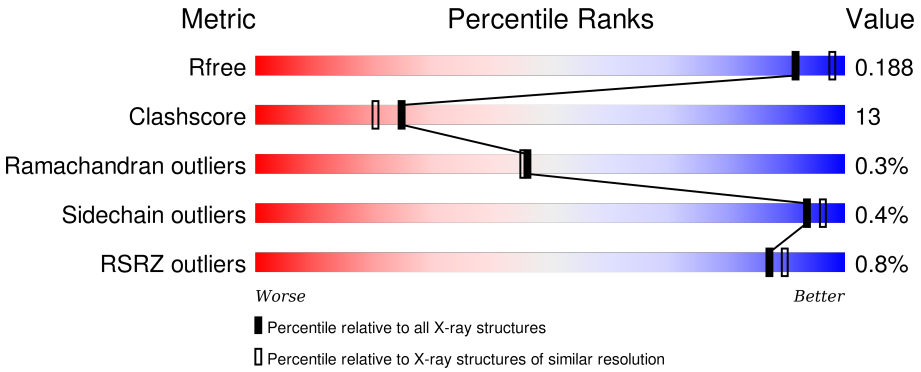
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	147	69% 24% 5%
1	B	147	69% 27%
1	C	147	78% 20%
1	D	147	74% 21% 5%
1	E	147	75% 20% 5%

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Mol	Chain	Length	Quality of chain
1	F	147	74% 22% •
1	G	147	2% 73% 21% • 5%
1	H	147	2% 73% 23% •
1	I	147	75% 20% • 5%
1	J	147	70% 25% 5%
1	K	147	% 71% 24% 5%
1	L	147	% 65% 28% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	B	402	-	-	-	X
2	CA	G	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14057 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 Pulmonary surfactant-associated protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1061	669	177	210	5			
1	B	142	Total	C	N	O	S	0	0	0
			1078	680	180	213	5			
1	C	144	Total	C	N	O	S	0	0	0
			1092	688	182	217	5			
1	D	140	Total	C	N	O	S	0	0	0
			1061	669	177	210	5			
1	E	140	Total	C	N	O	S	0	0	0
			1061	669	177	210	5			
1	F	141	Total	C	N	O	S	0	0	0
			1070	674	179	212	5			
1	G	140	Total	C	N	O	S	0	0	0
			1061	669	177	210	5			
1	H	142	Total	C	N	O	S	0	0	0
			1078	680	180	213	5			
1	I	140	Total	C	N	O	S	0	0	0
			1061	669	177	210	5			
1	J	140	Total	C	N	O	S	0	0	0
			1061	669	177	210	5			
1	K	139	Total	C	N	O	S	0	0	0
			1057	667	176	209	5			
1	L	138	Total	C	N	O	S	0	0	0
			1048	662	174	207	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
A	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
B	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
B	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
C	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247

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Chain	Residue	Modelled	Actual	Comment	Reference
C	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
D	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
D	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
E	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
E	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
F	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
F	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
G	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
G	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
H	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
H	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
I	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
I	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
J	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
J	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
K	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
K	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247
L	325	ALA	ASP	ENGINEERED MUTATION	UNP P35247
L	343	VAL	ARG	ENGINEERED MUTATION	UNP P35247

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Ca 3 3	0	0
2	J	3	Total Ca 3 3	0	0
2	D	3	Total Ca 3 3	0	0
2	K	3	Total Ca 3 3	0	0
2	E	3	Total Ca 3 3	0	0
2	H	3	Total Ca 3 3	0	0
2	B	3	Total Ca 3 3	0	0
2	I	3	Total Ca 3 3	0	0
2	C	3	Total Ca 3 3	0	0
2	A	3	Total Ca 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	3	Total Ca 3 3	0	0
2	F	3	Total Ca 3 3	0	0

- Molecule 3 is water.

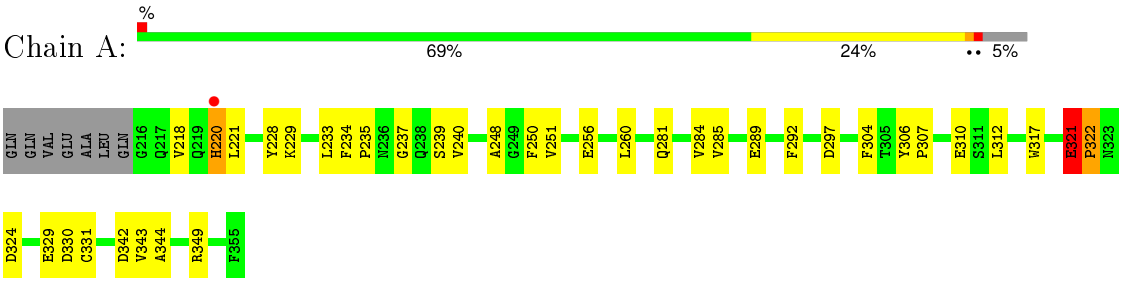
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	127	Total O 127 127	0	0
3	B	117	Total O 117 117	0	0
3	C	126	Total O 126 126	0	0
3	D	122	Total O 122 122	0	0
3	E	129	Total O 129 129	0	0
3	F	81	Total O 81 81	0	0
3	G	112	Total O 112 112	0	0
3	H	57	Total O 57 57	0	0
3	I	99	Total O 99 99	0	0
3	J	83	Total O 83 83	0	0
3	K	90	Total O 90 90	0	0
3	L	89	Total O 89 89	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 errors 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.

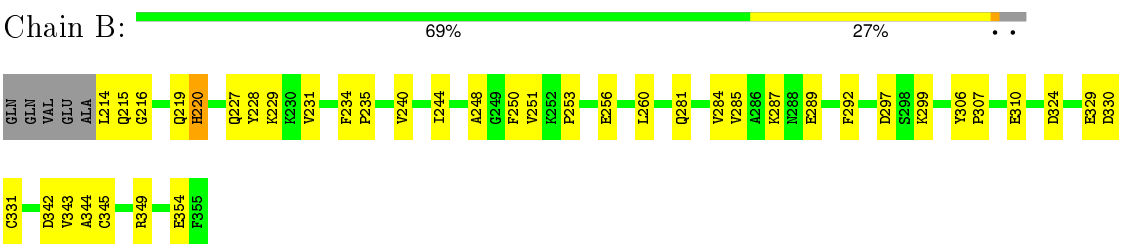
- Molecule 1: Pulmonary surfactant-associated protein D

Chain A:



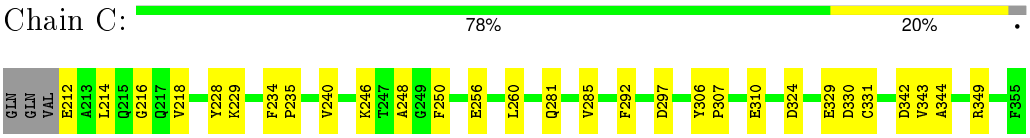
- Molecule 1: Pulmonary surfactant-associated protein D

Chain B:



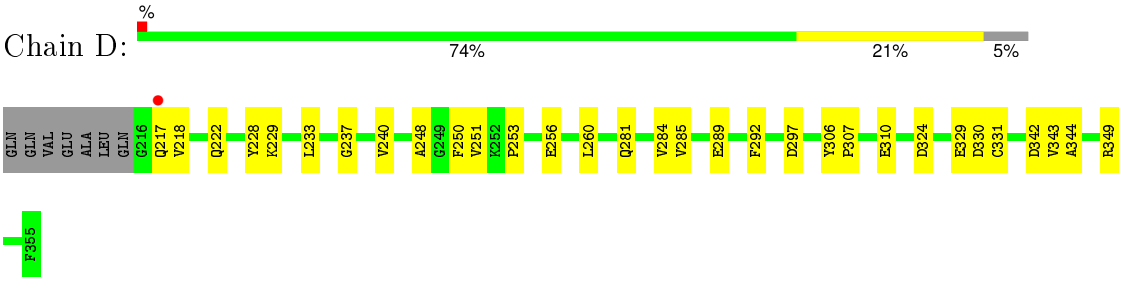
- Molecule 1: Pulmonary surfactant-associated protein D

Chain C:



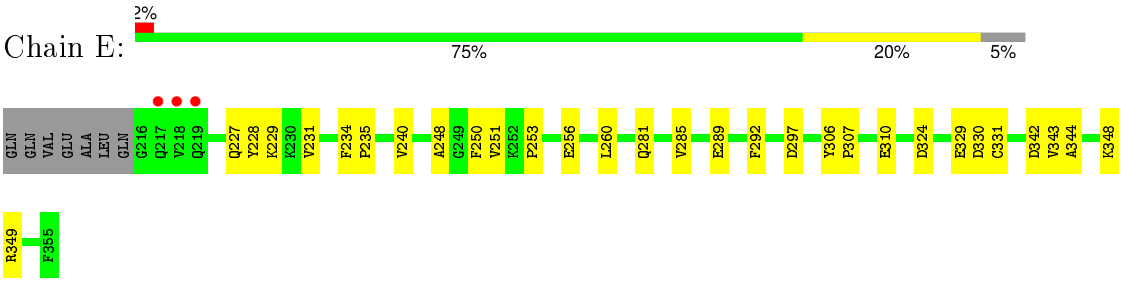
- Molecule 1: Pulmonary surfactant-associated protein D

Chain D:



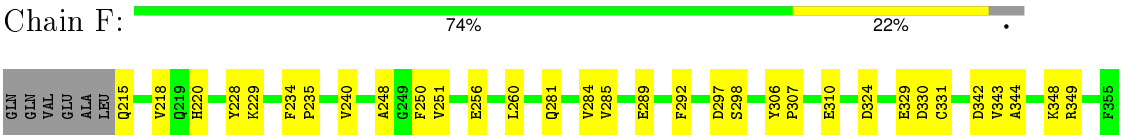
- Molecule 1: Pulmonary surfactant-associated protein D

Chain E:



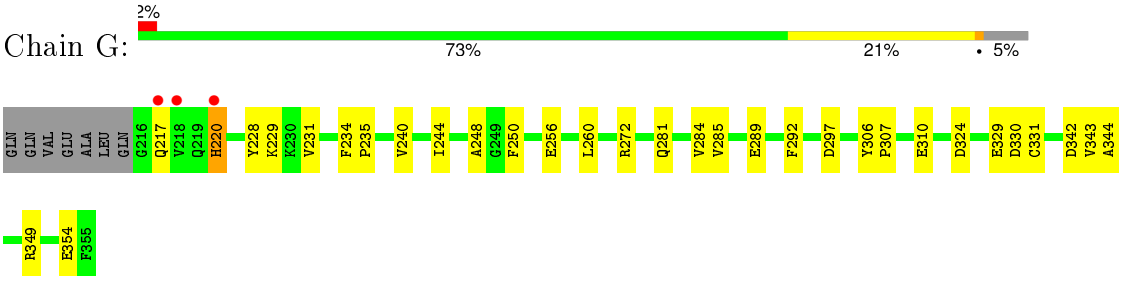
• Molecule 1: Pulmonary surfactant-associated protein D

Chain F:



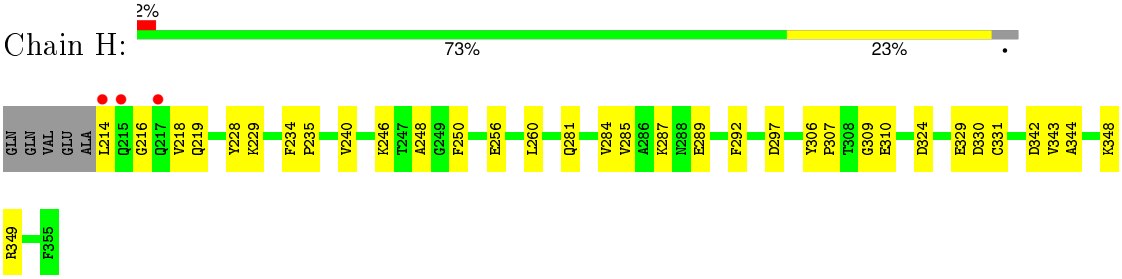
• Molecule 1: Pulmonary surfactant-associated protein D

Chain G:



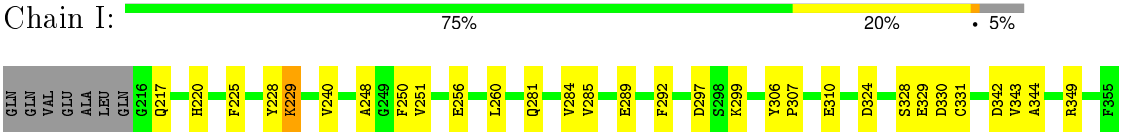
• Molecule 1: Pulmonary surfactant-associated protein D

Chain H:



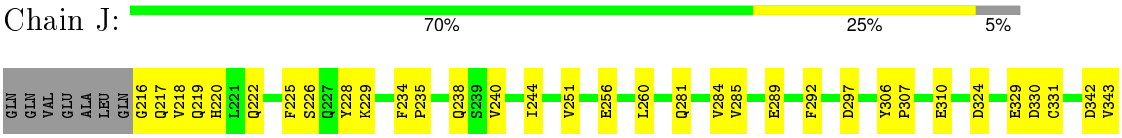
• Molecule 1: Pulmonary surfactant-associated protein D

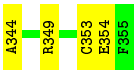
Chain I:



• Molecule 1: Pulmonary surfactant-associated protein D

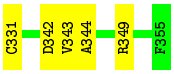
Chain J:





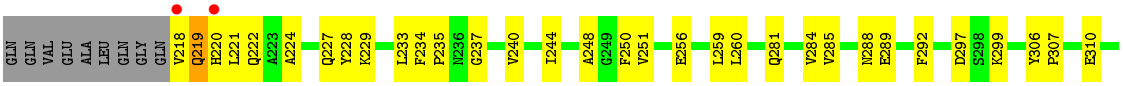
• Molecule 1: Pulmonary surfactant-associated protein D

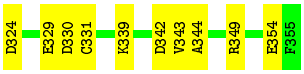
Chain K:



• Molecule 1: Pulmonary surfactant-associated protein D

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.52Å 160.11Å 160.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.94 – 2.10 14.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (14.94-2.10) 95.1 (14.94-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1063)	Depositor
R, R_{free}	0.163 , 0.188 0.163 , 0.188	Depositor DCC
R_{free} test set	2009 reflections (1.30%)	DCC
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 30.6	EDS
Estimated twinning fraction	0.490 for -h,l,k 0.469 for -h,l,k	Xtriage
Reported twinning fraction	0.490 for -h,l,k	Depositor
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 154598 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14057	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA

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	0.26	0/1083	0.41	0/1464
1	B	0.22	0/1100	0.37	0/1487
1	C	0.22	0/1114	0.38	0/1506
1	D	0.23	0/1083	0.37	0/1464
1	E	0.22	0/1083	0.36	0/1464
1	F	0.23	0/1092	0.38	0/1476
1	G	0.22	0/1083	0.37	0/1464
1	H	0.22	0/1100	0.37	0/1487
1	I	0.22	0/1083	0.37	0/1464
1	J	0.23	0/1083	0.37	0/1464
1	K	0.22	0/1079	0.37	0/1459
1	L	0.23	0/1070	0.38	0/1447
All	All	0.23	0/13053	0.37	0/17646

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	GLU	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	1061	0	1018	41	0
1	B	1078	0	1037	35	0
1	C	1092	0	1048	26	0
1	D	1061	0	1018	25	0
1	E	1061	0	1018	22	0
1	F	1070	0	1026	31	0
1	G	1061	0	1018	26	0
1	H	1078	0	1037	29	0
1	I	1061	0	1018	24	1
1	J	1061	0	1018	37	0
1	K	1057	0	1015	28	0
1	L	1048	0	1007	45	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	127	0	0	1	0
3	B	117	0	0	5	0
3	C	126	0	0	0	0
3	D	122	0	0	2	0
3	E	129	0	0	0	0
3	F	81	0	0	5	0
3	G	112	0	0	2	0
3	H	57	0	0	4	0
3	I	99	0	0	2	0
3	J	83	0	0	1	0
3	K	90	0	0	2	0
3	L	89	0	0	3	0
All	All	14057	0	12278	321	1

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 13.

All (321) 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:A:317:TRP:CE3	1:A:322:PRO:HD3	1.84	1.12
1:A:317:TRP:CD2	1:A:322:PRO:CD	2.52	0.92
1:A:317:TRP:CE3	1:A:322:PRO:CD	2.58	0.86
1:A:317:TRP:CD2	1:A:322:PRO:HD3	2.10	0.86
1:G:229:LYS:HG3	1:I:228:TYR:OH	1.80	0.81
1:B:228:TYR:CZ	1:C:229:LYS:HG3	2.18	0.78
1:J:218:VAL:HG22	1:L:218:VAL:HG22	1.65	0.78
1:A:321:GLU:O	1:A:322:PRO:O	2.02	0.78
1:A:317:TRP:CD2	1:A:322:PRO:HD2	2.18	0.77
1:J:228:TYR:OH	1:K:229:LYS:HG3	1.86	0.76
1:A:317:TRP:CZ3	1:A:322:PRO:HD3	2.21	0.76
1:J:218:VAL:CG2	1:L:218:VAL:HG22	2.15	0.76
1:J:226:SER:HA	1:J:229:LYS:HD2	1.71	0.73
1:G:217:GLN:HB3	1:G:220:HIS:HB3	1.70	0.72
1:F:215:GLN:HB3	1:F:218:VAL:HB	1.73	0.71
1:A:229:LYS:HG3	1:C:228:TYR:CZ	2.26	0.69
1:A:228:TYR:CZ	1:B:229:LYS:HG3	2.27	0.69
1:A:317:TRP:CG	1:A:322:PRO:HD2	2.28	0.68
1:G:229:LYS:HG3	1:I:228:TYR:CZ	2.29	0.68
1:L:218:VAL:O	1:L:221:LEU:N	2.28	0.67
1:B:214:LEU:HD23	1:B:215:GLN:N	2.10	0.67
1:J:225:PHE:O	1:J:229:LYS:HG3	1.95	0.67
1:J:225:PHE:HZ	1:L:228:TYR:CD2	2.14	0.66
1:H:256:GLU:OE1	3:H:508:HOH:O	2.13	0.66
1:K:228:TYR:CZ	1:L:229:LYS:HG3	2.31	0.66
1:A:229:LYS:HG3	1:C:228:TYR:CE1	2.31	0.65
1:H:228:TYR:CZ	1:I:229:LYS:HG2	2.33	0.64
1:J:216:GLY:O	1:J:219:GLN:HG2	1.98	0.64
1:A:229:LYS:HE2	1:C:228:TYR:CE2	2.32	0.64
1:E:228:TYR:CZ	1:F:229:LYS:HG3	2.31	0.64
1:L:224:ALA:O	1:L:228:TYR:HD2	1.80	0.63
1:F:220:HIS:ND1	1:F:220:HIS:O	2.30	0.63
1:D:253:PRO:HB2	3:H:508:HOH:O	1.97	0.63
1:E:292:PHE:CD2	1:E:349:ARG:HB2	2.35	0.62
1:K:226:SER:O	1:K:229:LYS:HB3	2.00	0.61
1:E:228:TYR:OH	1:F:229:LYS:HG3	2.00	0.61
1:D:228:TYR:CZ	1:E:229:LYS:HG3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LYS:NZ	1:D:289:GLU:OE2	2.34	0.60
1:A:289:GLU:HG3	3:A:543:HOH:O	2.01	0.60
1:H:306:TYR:HB3	1:H:307:PRO:HD2	1.84	0.59
1:J:225:PHE:CZ	1:L:228:TYR:CD2	2.90	0.59
1:I:256:GLU:O	1:I:260:LEU:HG	2.02	0.59
1:K:228:TYR:CE1	1:L:229:LYS:HG3	2.38	0.59
1:I:343:VAL:HG22	1:I:344:ALA:N	2.18	0.59
1:C:343:VAL:HG22	1:C:344:ALA:N	2.19	0.58
1:B:306:TYR:HB3	1:B:307:PRO:HD2	1.85	0.58
1:A:229:LYS:HE2	1:C:228:TYR:CZ	2.39	0.58
1:H:287:LYS:NZ	3:H:519:HOH:O	2.33	0.58
1:H:309:GLY:HA3	3:H:506:HOH:O	2.04	0.58
1:F:343:VAL:HG22	1:F:344:ALA:N	2.18	0.58
1:G:306:TYR:HB3	1:G:307:PRO:HD2	1.85	0.58
1:J:343:VAL:HG22	1:J:344:ALA:N	2.19	0.58
1:D:343:VAL:HG22	1:D:344:ALA:N	2.19	0.58
1:J:238:GLN:HA	3:J:558:HOH:O	2.04	0.58
1:K:343:VAL:HG22	1:K:344:ALA:N	2.19	0.57
1:E:227:GLN:O	1:E:231:VAL:HG23	2.04	0.57
1:J:220:HIS:O	1:J:220:HIS:ND1	2.36	0.57
1:G:343:VAL:HG22	1:G:344:ALA:N	2.20	0.57
1:D:229:LYS:HG3	1:F:228:TYR:OH	2.05	0.57
1:H:343:VAL:HG22	1:H:344:ALA:N	2.18	0.57
1:D:229:LYS:HG3	1:F:228:TYR:CZ	2.39	0.57
1:F:306:TYR:HB3	1:F:307:PRO:HD2	1.87	0.56
1:K:218:VAL:O	1:K:222:GLN:HG3	2.04	0.56
1:E:256:GLU:O	1:E:260:LEU:HG	2.05	0.56
1:C:306:TYR:HB3	1:C:307:PRO:HD2	1.87	0.56
1:J:229:LYS:HG2	1:L:228:TYR:CE1	2.39	0.56
1:L:292:PHE:CD2	1:L:349:ARG:HB2	2.40	0.56
1:L:306:TYR:HB3	1:L:307:PRO:HD2	1.87	0.56
1:I:306:TYR:HB3	1:I:307:PRO:HD2	1.88	0.56
1:A:306:TYR:HB3	1:A:307:PRO:HD2	1.88	0.56
1:A:228:TYR:CE1	1:B:229:LYS:HG3	2.41	0.56
1:L:343:VAL:HG22	1:L:344:ALA:N	2.21	0.56
1:F:220:HIS:C	1:F:220:HIS:HD1	2.10	0.55
1:K:292:PHE:CD2	1:K:349:ARG:HB2	2.42	0.55
1:H:216:GLY:HA2	1:H:219:GLN:NE2	2.21	0.55
1:I:324:ASP:HA	1:I:329:GLU:HB2	1.88	0.55
1:B:214:LEU:HD23	1:B:214:LEU:C	2.27	0.55
1:A:343:VAL:HG22	1:A:344:ALA:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:VAL:HG22	1:B:344:ALA:N	2.22	0.55
1:J:292:PHE:CD2	1:J:349:ARG:HB2	2.41	0.55
1:G:228:TYR:CZ	1:H:229:LYS:HG3	2.42	0.55
1:L:256:GLU:O	1:L:260:LEU:HG	2.07	0.55
1:F:324:ASP:HB2	3:F:501:HOH:O	2.06	0.54
1:B:297:ASP:OD1	1:B:330:ASP:HA	2.08	0.54
1:J:222:GLN:HG2	1:L:221:LEU:HD13	1.89	0.54
1:D:256:GLU:O	1:D:260:LEU:HG	2.07	0.54
1:C:256:GLU:O	1:C:260:LEU:HG	2.07	0.54
1:K:299:LYS:HD2	3:K:565:HOH:O	2.06	0.54
1:E:306:TYR:HB3	1:E:307:PRO:HD2	1.90	0.54
1:K:306:TYR:HB3	1:K:307:PRO:HD2	1.89	0.54
1:D:306:TYR:HB3	1:D:307:PRO:HD2	1.89	0.54
1:A:321:GLU:O	1:A:322:PRO:C	2.47	0.53
1:J:324:ASP:HA	1:J:329:GLU:HB2	1.90	0.53
1:F:324:ASP:CB	3:F:501:HOH:O	2.56	0.53
1:H:292:PHE:CD2	1:H:349:ARG:HB2	2.43	0.53
1:A:218:VAL:O	1:A:221:LEU:N	2.41	0.53
1:G:217:GLN:HB3	1:G:220:HIS:CB	2.37	0.53
1:G:292:PHE:CD2	1:G:349:ARG:HB2	2.43	0.53
1:J:306:TYR:HB3	1:J:307:PRO:HD2	1.89	0.53
1:D:289:GLU:HG3	3:D:540:HOH:O	2.09	0.53
1:E:343:VAL:HG22	1:E:344:ALA:N	2.23	0.53
1:J:256:GLU:O	1:J:260:LEU:HG	2.07	0.53
1:B:228:TYR:OH	1:C:229:LYS:HG3	2.07	0.53
1:I:225:PHE:CE2	1:I:229:LYS:HE3	2.44	0.53
1:L:259:LEU:HD12	3:L:555:HOH:O	2.09	0.53
1:F:256:GLU:O	1:F:260:LEU:HG	2.09	0.53
1:G:228:TYR:OH	1:H:229:LYS:HG3	2.09	0.52
1:A:297:ASP:OD1	1:A:330:ASP:HA	2.09	0.52
1:H:234:PHE:CE1	1:H:235:PRO:HB3	2.45	0.52
1:C:214:LEU:O	1:C:218:VAL:HG23	2.09	0.52
1:B:306:TYR:HD2	1:B:310:GLU:HG3	1.73	0.52
1:I:297:ASP:OD1	1:I:330:ASP:HA	2.10	0.52
1:L:324:ASP:HA	1:L:329:GLU:HB2	1.91	0.52
1:J:225:PHE:CD2	1:J:229:LYS:HE3	2.45	0.52
1:D:292:PHE:CD2	1:D:349:ARG:HB2	2.44	0.52
1:K:256:GLU:O	1:K:260:LEU:HG	2.09	0.52
1:B:227:GLN:O	1:B:231:VAL:HG23	2.09	0.51
1:A:284:VAL:HG13	1:A:289:GLU:O	2.10	0.51
1:L:250:PHE:CZ	1:L:260:LEU:HD13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:281:GLN:O	1:J:285:VAL:HG23	2.10	0.51
1:C:324:ASP:HA	1:C:329:GLU:HB2	1.93	0.51
1:B:256:GLU:O	1:B:260:LEU:HG	2.10	0.51
1:F:348:LYS:HE3	3:F:533:HOH:O	2.11	0.51
1:H:214:LEU:O	1:H:218:VAL:HG23	2.10	0.51
1:D:297:ASP:OD1	1:D:330:ASP:HA	2.11	0.51
1:J:353:CYS:SG	1:L:234:PHE:CZ	3.04	0.51
1:C:297:ASP:OD1	1:C:330:ASP:HA	2.11	0.50
1:A:229:LYS:HG3	1:C:228:TYR:OH	2.11	0.50
1:H:256:GLU:O	1:H:260:LEU:HG	2.11	0.50
1:A:292:PHE:CD2	1:A:349:ARG:HB2	2.47	0.50
1:G:297:ASP:OD1	1:G:330:ASP:HA	2.11	0.50
1:C:281:GLN:O	1:C:285:VAL:HG23	2.11	0.50
1:H:324:ASP:HA	1:H:329:GLU:HB2	1.94	0.50
1:H:297:ASP:OD1	1:H:330:ASP:HA	2.12	0.50
1:I:240:VAL:O	1:I:240:VAL:HG13	2.12	0.50
1:E:228:TYR:CE1	1:F:229:LYS:HG3	2.47	0.50
1:L:233:LEU:O	1:L:237:GLY:N	2.37	0.50
1:F:292:PHE:CD2	1:F:349:ARG:HB2	2.47	0.50
1:D:228:TYR:OH	1:E:229:LYS:HG3	2.12	0.50
1:L:297:ASP:OD1	1:L:330:ASP:HA	2.12	0.50
1:G:231:VAL:HG13	1:H:246:LYS:HD2	1.93	0.50
1:G:220:HIS:HD1	1:G:220:HIS:C	2.15	0.49
1:E:281:GLN:O	1:E:285:VAL:HG23	2.12	0.49
1:B:253:PRO:HG2	1:E:253:PRO:HG2	1.95	0.49
1:D:324:ASP:HA	1:D:329:GLU:HB2	1.94	0.49
1:J:297:ASP:OD1	1:J:330:ASP:HA	2.12	0.49
1:E:297:ASP:OD1	1:E:330:ASP:HA	2.12	0.49
1:A:256:GLU:O	1:A:260:LEU:HG	2.12	0.49
1:B:284:VAL:HG13	1:B:289:GLU:O	2.12	0.49
1:K:281:GLN:O	1:K:285:VAL:HG23	2.12	0.49
1:E:324:ASP:HA	1:E:329:GLU:HB2	1.95	0.49
1:F:298:SER:N	3:F:572:HOH:O	2.45	0.49
1:G:256:GLU:O	1:G:260:LEU:HG	2.12	0.49
1:A:281:GLN:O	1:A:285:VAL:HG23	2.12	0.48
1:I:331:CYS:O	1:I:342:ASP:HA	2.14	0.48
1:K:297:ASP:OD1	1:K:330:ASP:HA	2.13	0.48
1:H:228:TYR:CE1	1:I:229:LYS:HG2	2.49	0.48
1:G:284:VAL:HG13	1:G:289:GLU:O	2.12	0.48
1:I:292:PHE:CD2	1:I:349:ARG:HB2	2.48	0.48
1:A:228:TYR:OH	1:B:229:LYS:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:216:GLY:O	1:H:219:GLN:HG2	2.14	0.48
1:B:292:PHE:CD2	1:B:349:ARG:HB2	2.49	0.48
1:H:240:VAL:HG13	1:H:240:VAL:O	2.14	0.48
1:G:324:ASP:HA	1:G:329:GLU:HB2	1.95	0.48
1:D:218:VAL:HG12	1:D:222:GLN:HG3	1.95	0.48
1:H:281:GLN:O	1:H:285:VAL:HG23	2.13	0.48
1:B:324:ASP:HA	1:B:329:GLU:HB2	1.95	0.48
1:G:272:ARG:HD3	3:G:552:HOH:O	2.13	0.48
1:A:306:TYR:HD2	1:A:310:GLU:HG3	1.78	0.48
1:H:284:VAL:HG13	1:H:289:GLU:O	2.14	0.48
1:I:281:GLN:O	1:I:285:VAL:HG23	2.14	0.48
1:L:281:GLN:O	1:L:285:VAL:HG23	2.13	0.48
1:F:281:GLN:O	1:F:285:VAL:HG23	2.14	0.47
1:D:229:LYS:HG3	1:F:228:TYR:CE1	2.50	0.47
1:J:218:VAL:HG21	1:L:218:VAL:HG22	1.95	0.47
1:A:248:ALA:HB1	1:A:250:PHE:CE2	2.50	0.47
1:A:240:VAL:HG13	1:A:240:VAL:O	2.15	0.47
1:L:218:VAL:O	1:L:220:HIS:N	2.48	0.47
1:J:229:LYS:HG2	1:L:228:TYR:CZ	2.49	0.47
1:I:248:ALA:HB1	1:I:250:PHE:CE2	2.50	0.47
3:B:522:HOH:O	1:E:348:LYS:HE3	2.14	0.47
1:G:240:VAL:O	1:G:240:VAL:HG13	2.15	0.47
1:G:234:PHE:HA	1:G:235:PRO:HA	1.68	0.47
1:G:281:GLN:O	1:G:285:VAL:HG23	2.14	0.47
1:K:324:ASP:HA	1:K:329:GLU:HB2	1.97	0.47
1:K:228:TYR:CE2	1:L:244:ILE:HD11	2.50	0.47
1:J:306:TYR:HD2	1:J:310:GLU:HG3	1.80	0.47
3:D:542:HOH:O	1:H:348:LYS:HE2	2.14	0.47
1:A:324:ASP:HA	1:A:329:GLU:HB2	1.97	0.47
1:L:306:TYR:HD2	1:L:310:GLU:HG3	1.80	0.46
1:J:240:VAL:HG13	1:J:240:VAL:O	2.16	0.46
1:K:221:LEU:HD22	1:L:222:GLN:HG3	1.98	0.46
1:F:240:VAL:HG13	1:F:240:VAL:O	2.16	0.46
1:B:216:GLY:HA2	1:B:219:GLN:OE1	2.13	0.46
1:B:234:PHE:HA	1:B:235:PRO:HA	1.70	0.46
1:L:248:ALA:CB	1:L:250:PHE:CE2	2.99	0.46
1:F:324:ASP:HA	1:F:329:GLU:HB2	1.96	0.46
1:K:306:TYR:HD2	1:K:310:GLU:HG3	1.80	0.46
1:E:248:ALA:HB1	1:E:250:PHE:CE2	2.50	0.46
1:E:240:VAL:O	1:E:240:VAL:HG13	2.16	0.46
1:L:331:CYS:O	1:L:342:ASP:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ALA:HB1	1:B:250:PHE:CE2	2.51	0.46
1:C:248:ALA:HB1	1:C:250:PHE:CE2	2.51	0.46
1:G:306:TYR:HB3	1:G:307:PRO:CD	2.46	0.46
1:D:240:VAL:O	1:D:240:VAL:HG13	2.16	0.46
1:I:328:SER:HB2	3:I:546:HOH:O	2.16	0.46
1:B:240:VAL:O	1:B:240:VAL:HG13	2.16	0.46
1:C:331:CYS:O	1:C:342:ASP:HA	2.15	0.45
1:F:248:ALA:HB1	1:F:250:PHE:CE2	2.52	0.45
1:I:306:TYR:HB3	1:I:307:PRO:CD	2.46	0.45
1:G:331:CYS:O	1:G:342:ASP:HA	2.17	0.45
1:F:284:VAL:HG13	1:F:289:GLU:O	2.16	0.45
1:B:289:GLU:HG3	3:B:519:HOH:O	2.16	0.45
1:K:234:PHE:HA	1:K:235:PRO:HA	1.71	0.45
1:I:225:PHE:CE2	1:I:229:LYS:CE	3.00	0.45
1:F:229:LYS:HD2	3:F:524:HOH:O	2.17	0.45
1:I:284:VAL:HG13	1:I:289:GLU:O	2.16	0.45
1:H:331:CYS:O	1:H:342:ASP:HA	2.17	0.45
1:B:331:CYS:O	1:B:342:ASP:HA	2.17	0.45
1:A:331:CYS:O	1:A:342:ASP:HA	2.17	0.45
1:J:226:SER:HA	1:J:229:LYS:CD	2.43	0.45
1:L:306:TYR:HB3	1:L:307:PRO:CD	2.46	0.45
1:I:306:TYR:HD2	1:I:310:GLU:HG3	1.81	0.45
1:E:306:TYR:HD2	1:E:310:GLU:HG3	1.81	0.45
1:B:220:HIS:HD1	1:B:220:HIS:C	2.21	0.45
1:J:343:VAL:CG2	1:J:344:ALA:N	2.80	0.45
1:F:306:TYR:HD2	1:F:310:GLU:HG3	1.82	0.45
1:C:306:TYR:HB3	1:C:307:PRO:CD	2.47	0.45
1:D:233:LEU:O	1:D:237:GLY:N	2.49	0.45
1:A:322:PRO:HA	1:A:342:ASP:CG	2.38	0.44
1:F:220:HIS:C	1:F:220:HIS:ND1	2.69	0.44
1:I:343:VAL:CG2	1:I:344:ALA:N	2.81	0.44
1:J:331:CYS:O	1:J:342:ASP:HA	2.16	0.44
1:D:281:GLN:O	1:D:285:VAL:HG23	2.17	0.44
1:B:234:PHE:O	1:C:246:LYS:NZ	2.48	0.44
1:A:220:HIS:HD1	1:A:220:HIS:C	2.19	0.44
1:D:284:VAL:HG13	1:D:289:GLU:O	2.17	0.44
1:D:248:ALA:HB1	1:D:250:PHE:CE2	2.52	0.44
1:B:281:GLN:O	1:B:285:VAL:HG23	2.17	0.44
1:G:306:TYR:HD2	1:G:310:GLU:HG3	1.83	0.44
1:D:343:VAL:CG2	1:D:344:ALA:N	2.81	0.44
1:C:292:PHE:CD2	1:C:349:ARG:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:ASP:OD1	1:F:330:ASP:HA	2.17	0.44
1:D:306:TYR:HB3	1:D:307:PRO:CD	2.47	0.44
1:E:331:CYS:O	1:E:342:ASP:HA	2.17	0.44
1:J:244:ILE:O	1:J:354:GLU:HA	2.18	0.44
1:B:287:LYS:HG2	3:B:550:HOH:O	2.17	0.44
1:D:331:CYS:O	1:D:342:ASP:HA	2.18	0.44
1:J:218:VAL:HG21	1:L:218:VAL:CG2	2.47	0.44
1:L:224:ALA:O	1:L:228:TYR:CD2	2.66	0.44
1:J:220:HIS:HD1	1:J:220:HIS:C	2.19	0.44
1:C:212:GLU:C	1:C:214:LEU:H	2.19	0.44
1:H:306:TYR:HB3	1:H:307:PRO:CD	2.48	0.44
1:I:217:GLN:O	1:I:220:HIS:HB3	2.18	0.44
1:K:343:VAL:CG2	1:K:344:ALA:N	2.81	0.43
1:K:240:VAL:O	1:K:240:VAL:HG13	2.18	0.43
1:G:248:ALA:HB1	1:G:250:PHE:CE2	2.53	0.43
1:F:343:VAL:CG2	1:F:344:ALA:N	2.80	0.43
1:K:306:TYR:HB3	1:K:307:PRO:CD	2.48	0.43
1:G:343:VAL:CG2	1:G:344:ALA:N	2.81	0.43
1:C:306:TYR:HD2	1:C:310:GLU:HG3	1.83	0.43
1:L:234:PHE:HA	1:L:235:PRO:HA	1.74	0.43
1:L:284:VAL:HG13	1:L:289:GLU:O	2.18	0.43
1:B:345:CYS:HB2	3:B:553:HOH:O	2.18	0.43
1:H:306:TYR:HD2	1:H:310:GLU:HG3	1.84	0.43
1:D:306:TYR:HD2	1:D:310:GLU:HG3	1.83	0.43
1:B:251:VAL:CG1	1:B:289:GLU:HG2	2.49	0.43
1:H:248:ALA:HB1	1:H:250:PHE:CE2	2.53	0.43
1:L:299:LYS:HD2	3:L:521:HOH:O	2.19	0.43
1:C:343:VAL:CG2	1:C:344:ALA:N	2.81	0.43
1:E:234:PHE:HA	1:E:235:PRO:HA	1.70	0.43
1:L:218:VAL:O	1:L:219:GLN:C	2.57	0.42
1:F:306:TYR:HB3	1:F:307:PRO:CD	2.48	0.42
1:J:306:TYR:HB3	1:J:307:PRO:CD	2.50	0.42
1:J:234:PHE:HA	1:J:235:PRO:HA	1.68	0.42
1:K:248:ALA:HB1	1:K:250:PHE:CE2	2.54	0.42
1:L:251:VAL:HG11	1:L:289:GLU:HG2	2.01	0.42
1:J:284:VAL:HG13	1:J:289:GLU:O	2.20	0.42
1:F:234:PHE:HA	1:F:235:PRO:HA	1.73	0.42
1:K:331:CYS:O	1:K:342:ASP:HA	2.19	0.42
1:L:339:LYS:HG3	3:L:529:HOH:O	2.19	0.42
1:B:299:LYS:HD2	3:B:568:HOH:O	2.18	0.42
1:B:244:ILE:O	1:B:354:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:PHE:HA	1:C:235:PRO:HA	1.74	0.42
1:I:251:VAL:CG1	1:I:289:GLU:HG2	2.49	0.42
1:H:343:VAL:CG2	1:H:344:ALA:N	2.81	0.42
1:F:331:CYS:O	1:F:342:ASP:HA	2.19	0.42
1:L:343:VAL:CG2	1:L:344:ALA:N	2.83	0.42
1:A:304:PHE:O	1:A:312:LEU:HD13	2.19	0.42
1:J:228:TYR:CZ	1:K:229:LYS:HG3	2.54	0.42
1:B:228:TYR:CE1	1:C:229:LYS:HG3	2.54	0.41
1:A:306:TYR:HB3	1:A:307:PRO:CD	2.48	0.41
1:H:234:PHE:HA	1:H:235:PRO:HA	1.72	0.41
1:I:289:GLU:HG3	3:I:521:HOH:O	2.21	0.41
1:A:343:VAL:CG2	1:A:344:ALA:N	2.84	0.41
1:K:221:LEU:CD2	1:L:222:GLN:HG3	2.51	0.41
1:L:251:VAL:HG23	1:L:251:VAL:O	2.19	0.41
1:K:304:PHE:O	1:K:312:LEU:HD13	2.20	0.41
1:G:244:ILE:O	1:G:354:GLU:HA	2.20	0.41
1:H:216:GLY:HA2	1:H:219:GLN:HE21	1.85	0.41
1:B:343:VAL:CG2	1:B:344:ALA:N	2.83	0.41
1:L:224:ALA:O	1:L:227:GLN:HB3	2.21	0.41
1:A:248:ALA:HB2	1:C:234:PHE:CZ	2.55	0.41
1:G:250:PHE:HB2	3:G:540:HOH:O	2.20	0.41
1:L:240:VAL:HG13	1:L:240:VAL:O	2.20	0.41
1:C:240:VAL:O	1:C:240:VAL:HG13	2.21	0.41
1:A:233:LEU:HD11	1:A:239:SER:HB3	2.03	0.41
1:J:228:TYR:CD2	1:K:225:PHE:HZ	2.39	0.41
1:L:248:ALA:HB1	1:L:250:PHE:CE2	2.56	0.41
1:E:251:VAL:CG1	1:E:289:GLU:HG2	2.50	0.41
1:A:234:PHE:HA	1:A:235:PRO:HA	1.69	0.40
1:K:289:GLU:HG3	3:K:520:HOH:O	2.21	0.40
1:B:306:TYR:HB3	1:B:307:PRO:CD	2.51	0.40
1:J:251:VAL:CG1	1:J:289:GLU:HG2	2.52	0.40
1:D:251:VAL:CG1	1:D:289:GLU:HG2	2.50	0.40
1:A:251:VAL:CG1	1:A:289:GLU:HG2	2.51	0.40
1:A:233:LEU:O	1:A:237:GLY:N	2.52	0.40
1:L:244:ILE:O	1:L:354:GLU:HA	2.21	0.40
1:K:284:VAL:HG13	1:K:289:GLU:O	2.21	0.40
1:E:306:TYR:HB3	1:E:307:PRO:CD	2.50	0.40
1:F:251:VAL:CG1	1:F:289:GLU:HG2	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:299:LYS:NZ	1:L:288:ASN:O[2_355]	2.09	0.11

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	138/147 (94%)	133 (96%)	3 (2%)	2 (1%)	14 7
1	B	140/147 (95%)	137 (98%)	3 (2%)	0	100 100
1	C	142/147 (97%)	137 (96%)	4 (3%)	1 (1%)	26 21
1	D	138/147 (94%)	134 (97%)	4 (3%)	0	100 100
1	E	138/147 (94%)	135 (98%)	3 (2%)	0	100 100
1	F	139/147 (95%)	136 (98%)	3 (2%)	0	100 100
1	G	138/147 (94%)	135 (98%)	3 (2%)	0	100 100
1	H	140/147 (95%)	137 (98%)	3 (2%)	0	100 100
1	I	138/147 (94%)	135 (98%)	3 (2%)	0	100 100
1	J	138/147 (94%)	132 (96%)	5 (4%)	1 (1%)	26 21
1	K	137/147 (93%)	132 (96%)	5 (4%)	0	100 100
1	L	136/147 (92%)	131 (96%)	4 (3%)	1 (1%)	26 21
All	All	1662/1764 (94%)	1614 (97%)	43 (3%)	5 (0%)	46 45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	GLU
1	A	322	PRO
1	L	219	GLN
1	J	217	GLN
1	C	216	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	111/117 (95%)	110 (99%)	1 (1%)	84 89
1	B	113/117 (97%)	112 (99%)	1 (1%)	84 89
1	C	114/117 (97%)	114 (100%)	0	100 100
1	D	111/117 (95%)	110 (99%)	1 (1%)	84 89
1	E	111/117 (95%)	111 (100%)	0	100 100
1	F	112/117 (96%)	112 (100%)	0	100 100
1	G	111/117 (95%)	110 (99%)	1 (1%)	84 89
1	H	113/117 (97%)	113 (100%)	0	100 100
1	I	111/117 (95%)	110 (99%)	1 (1%)	84 89
1	J	111/117 (95%)	111 (100%)	0	100 100
1	K	111/117 (95%)	110 (99%)	1 (1%)	84 89
1	L	110/117 (94%)	110 (100%)	0	100 100
All	All	1339/1404 (95%)	1333 (100%)	6 (0%)	93 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	HIS
1	B	220	HIS
1	D	217	GLN
1	G	220	HIS
1	I	229	LYS
1	K	220	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	227	GLN
1	H	219	GLN
1	I	288	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

Of 36 ligands modelled in this entry, 36 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 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	140/147 (95%)	-0.54	1 (0%) 89 91	18, 23, 39, 90	0
1	B	142/147 (96%)	-0.58	0 100 100	18, 24, 45, 57	0
1	C	144/147 (97%)	-0.54	0 100 100	19, 25, 53, 74	0
1	D	140/147 (95%)	-0.55	1 (0%) 89 91	19, 25, 45, 93	0
1	E	140/147 (95%)	-0.53	3 (2%) 67 72	17, 24, 42, 84	0
1	F	141/147 (95%)	-0.51	0 100 100	21, 30, 49, 78	0
1	G	140/147 (95%)	-0.52	3 (2%) 67 72	20, 25, 50, 87	0
1	H	142/147 (96%)	-0.43	3 (2%) 67 72	23, 34, 49, 74	0
1	I	140/147 (95%)	-0.51	0 100 100	21, 29, 44, 77	0
1	J	140/147 (95%)	-0.51	0 100 100	21, 29, 52, 75	0
1	K	139/147 (94%)	-0.55	1 (0%) 89 91	21, 27, 49, 68	0
1	L	138/147 (93%)	-0.47	2 (1%) 78 82	21, 28, 43, 96	0
All	All	1686/1764 (95%)	-0.52	14 (0%) 87 90	17, 27, 50, 96	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	217	GLN	3.7
1	H	214	LEU	3.5
1	L	218	VAL	3.2
1	G	218	VAL	3.2
1	H	217	GLN	3.1
1	H	215	GLN	3.0
1	L	220	HIS	2.6
1	D	217	GLN	2.5
1	G	217	GLN	2.4
1	E	218	VAL	2.4
1	A	220	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	217	GLN	2.2
1	G	220	HIS	2.2
1	E	219	GLN	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CA	G	401	1/1	0.99	0.12	3.20	28,28,28,28	0
2	CA	B	402	1/1	0.98	0.10	2.81	31,31,31,31	0
2	CA	L	402	1/1	0.99	0.10	1.66	36,36,36,36	0
2	CA	E	401	1/1	0.99	0.10	1.53	27,27,27,27	0
2	CA	E	402	1/1	0.98	0.10	1.41	26,26,26,26	0
2	CA	D	402	1/1	0.99	0.08	0.51	33,33,33,33	0
2	CA	D	401	1/1	0.99	0.09	0.42	29,29,29,29	0
2	CA	C	401	1/1	0.99	0.09	0.34	29,29,29,29	0
2	CA	K	402	1/1	0.97	0.09	0.32	34,34,34,34	0
2	CA	A	401	1/1	0.99	0.09	0.20	26,26,26,26	0
2	CA	K	401	1/1	0.98	0.08	0.04	32,32,32,32	0
2	CA	I	402	1/1	0.99	0.08	-0.58	35,35,35,35	0
2	CA	B	401	1/1	0.94	0.07	-0.72	27,27,27,27	0
2	CA	F	401	1/1	0.97	0.06	-0.79	36,36,36,36	0
2	CA	F	403	1/1	0.93	0.06	-0.82	45,45,45,45	0
2	CA	I	401	1/1	0.97	0.07	-0.92	34,34,34,34	0
2	CA	G	402	1/1	0.99	0.07	-1.05	31,31,31,31	0
2	CA	J	401	1/1	0.97	0.06	-1.35	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	J	402	1/1	0.98	0.05	-2.32	40,40,40,40	0
2	CA	F	402	1/1	0.96	0.04	-2.36	46,46,46,46	0
2	CA	C	402	1/1	0.98	0.07	-2.39	31,31,31,31	0
2	CA	H	401	1/1	0.99	0.03	-2.82	41,41,41,41	0
2	CA	H	402	1/1	0.98	0.05	-2.87	39,39,39,39	0
2	CA	L	401	1/1	0.96	0.06	-2.88	36,36,36,36	0
2	CA	A	402	1/1	0.99	0.06	-3.13	27,27,27,27	0
2	CA	D	403	1/1	0.97	0.06	-	32,32,32,32	0
2	CA	A	403	1/1	0.97	0.09	-	30,30,30,30	0
2	CA	J	403	1/1	0.93	0.06	-	49,49,49,49	0
2	CA	H	403	1/1	0.96	0.04	-	43,43,43,43	0
2	CA	G	403	1/1	0.96	0.09	-	32,32,32,32	0
2	CA	L	403	1/1	0.97	0.08	-	32,32,32,32	0
2	CA	B	403	1/1	0.97	0.05	-	34,34,34,34	0
2	CA	K	403	1/1	0.98	0.08	-	35,35,35,35	0
2	CA	I	403	1/1	0.91	0.08	-	40,40,40,40	0
2	CA	E	403	1/1	0.92	0.08	-	30,30,30,30	0
2	CA	C	403	1/1	0.95	0.09	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.