Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 03:51 PM EDT

PDB ID	:	3BSQ
Title	:	Crystal structure of human kallikrein 7 produced as a secretion protein in E.coli
Authors	:	Fernandez, I.S.; Standker, L.; Magert, H.J.; Forssmann, W.G.; Gimenez-Gallego, G.; Romero, A.
Deposited on	:	2007-12-26
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

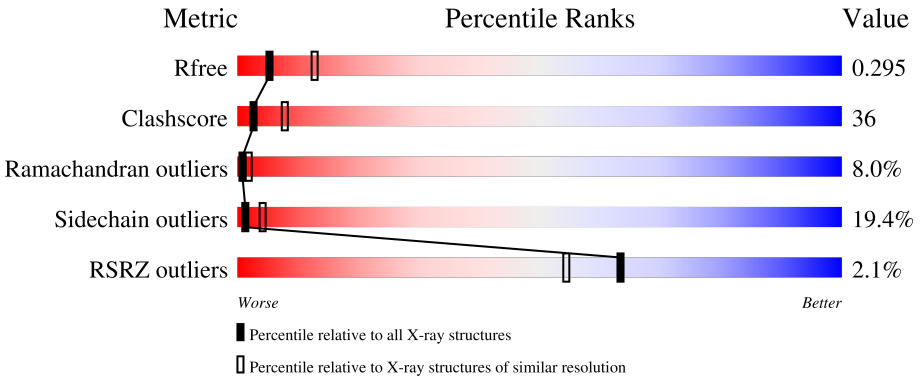
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	227	% 52% 28% 12% 6%
1	B	227	% 45% 33% 13% 5%
1	C	227	4% 51% 30% 9% 9%

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	SO4	B	14	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5148 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.

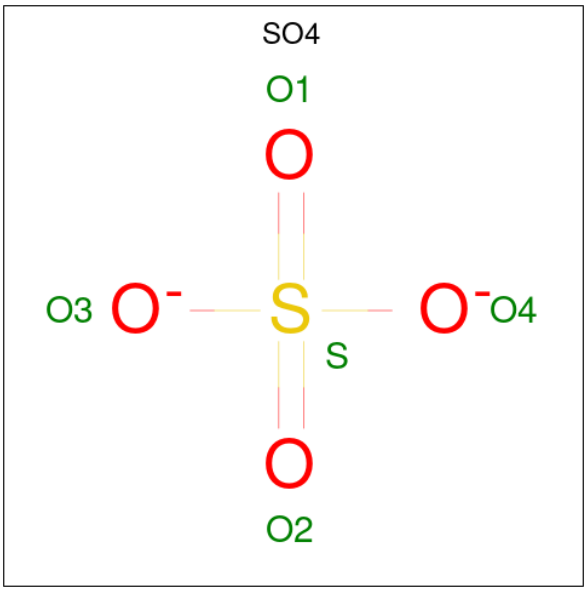
- Molecule 1 is a protein called Kallikrein-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1679	1045	300	316	18			
1	B	221	Total	C	N	O	S	0	0	0
			1664	1034	298	314	18			
1	C	223	Total	C	N	O	S	0	0	0
			1695	1054	307	316	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	HIS	-	expression tag	UNP P49862
A	238	HIS	-	expression tag	UNP P49862
A	239	HIS	-	expression tag	UNP P49862
A	240	HIS	-	expression tag	UNP P49862
A	241	HIS	-	expression tag	UNP P49862
A	242	HIS	-	expression tag	UNP P49862
B	237	HIS	-	expression tag	UNP P49862
B	238	HIS	-	expression tag	UNP P49862
B	239	HIS	-	expression tag	UNP P49862
B	240	HIS	-	expression tag	UNP P49862
B	241	HIS	-	expression tag	UNP P49862
B	242	HIS	-	expression tag	UNP P49862
C	237	HIS	-	expression tag	UNP P49862
C	238	HIS	-	expression tag	UNP P49862
C	239	HIS	-	expression tag	UNP P49862
C	240	HIS	-	expression tag	UNP P49862
C	241	HIS	-	expression tag	UNP P49862
C	242	HIS	-	expression tag	UNP P49862

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

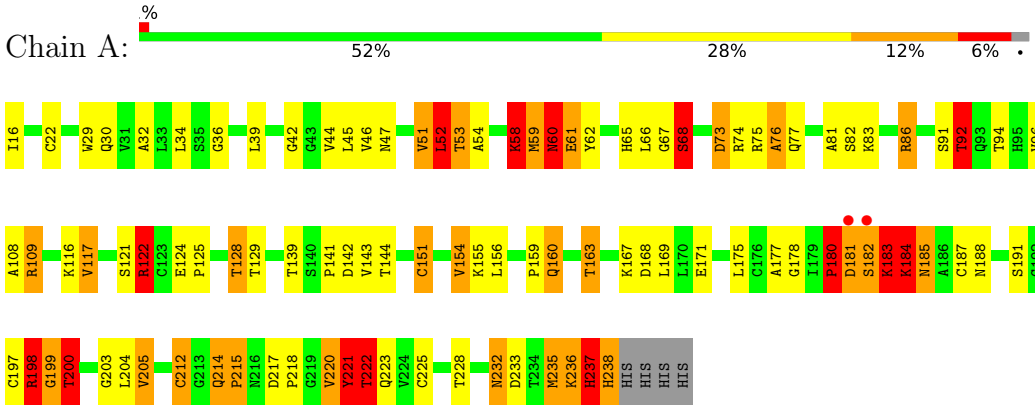
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	6	Total O 6 6	0	0
3	C	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

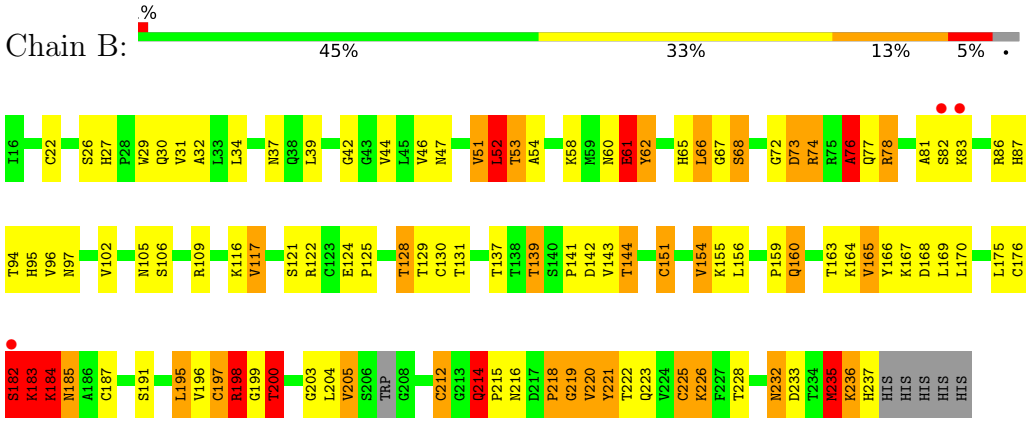
• Molecule 1: Kallikrein-7

Chain A:



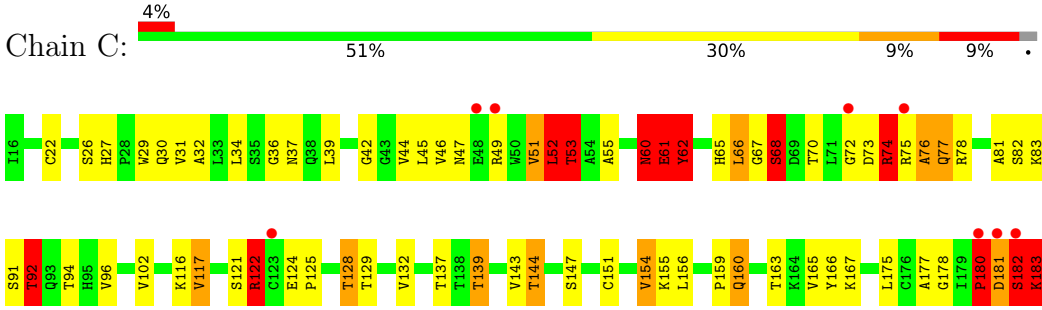
• Molecule 1: Kallikrein-7

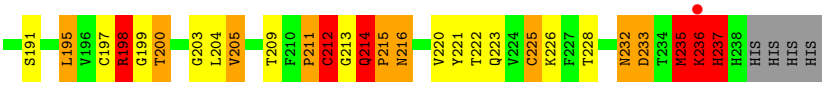
Chain B:



• Molecule 1: Kallikrein-7

Chain C:




S191
L195
V196
C197
R198
G199
T200
G203
L204
V205
T209
F210
P211
C212
G213
Q214
P215
N216
V220
Y221
T222
Q223
V224
C225
K226
F227
T228
N232
D233
T234
M235
K236
H237
H238
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	113.58Å 113.58Å 326.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 54.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.80) 98.4 (54.39-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.291 0.258 , 0.295	Depositor DCC
R_{free} test set	1027 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5148	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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: SO4

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	0.72	2/1718 (0.1%)	1.19	21/2337 (0.9%)
1	B	0.76	3/1699 (0.2%)	1.26	20/2305 (0.9%)
1	C	0.75	2/1734 (0.1%)	1.14	21/2355 (0.9%)
All	All	0.74	7/5151 (0.1%)	1.20	62/6997 (0.9%)

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	10
1	B	0	9
1	C	3	14
All	All	3	33

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	CYS	CB-SG	-7.24	1.70	1.82
1	C	60	ASN	CB-CG	5.88	1.64	1.51
1	A	151	CYS	CB-SG	-5.52	1.72	1.81
1	A	212	CYS	CB-SG	-5.49	1.72	1.81
1	B	225	CYS	CB-SG	-5.37	1.73	1.81
1	C	225	CYS	CB-SG	-5.16	1.73	1.81
1	B	151	CYS	CB-SG	-5.13	1.73	1.81

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	122	ARG	NE-CZ-NH1	-16.44	112.08	120.30
1	B	122	ARG	NE-CZ-NH2	15.54	128.07	120.30
1	A	122	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	C	52	LEU	C-N-CA	9.06	144.36	121.70
1	A	60	ASN	N-CA-CB	8.57	126.02	110.60
1	C	236	LYS	CD-CE-NZ	8.19	130.53	111.70
1	A	195	LEU	C-N-CA	8.01	141.71	121.70
1	A	58	LYS	C-N-CA	7.78	141.14	121.70
1	B	195	LEU	C-N-CA	7.78	141.14	121.70
1	A	220	VAL	C-N-CA	7.73	141.02	121.70
1	C	235	MET	C-N-CA	7.53	140.51	121.70
1	B	220	VAL	C-N-CA	7.05	139.34	121.70
1	B	122	ARG	CD-NE-CZ	6.87	133.22	123.60
1	B	197	CYS	CA-CB-SG	6.51	125.71	114.00
1	B	51	VAL	N-CA-C	-6.46	93.55	111.00
1	A	22	CYS	CA-CB-SG	6.32	125.38	114.00
1	C	61	GLU	C-N-CA	6.25	137.33	121.70
1	C	51	VAL	C-N-CA	6.24	137.31	121.70
1	C	51	VAL	N-CA-C	-6.02	94.75	111.00
1	A	122	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	51	VAL	C-N-CA	5.93	136.52	121.70
1	A	195	LEU	CA-CB-CG	5.91	128.90	115.30
1	B	51	VAL	C-N-CA	5.88	136.40	121.70
1	C	233	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	195	LEU	N-CA-C	-5.85	95.21	111.00
1	A	220	VAL	CA-C-N	5.78	129.93	117.20
1	C	236	LYS	CB-CG-CD	5.77	126.60	111.60
1	C	53	THR	N-CA-C	5.76	126.56	111.00
1	A	73	ASP	CA-C-N	5.73	129.81	117.20
1	B	195	LEU	CA-CB-CG	5.73	128.48	115.30
1	B	73	ASP	N-CA-C	-5.68	95.66	111.00
1	A	59	MET	C-N-CA	5.66	135.85	121.70
1	B	218	PRO	C-N-CA	5.64	134.15	122.30
1	A	235	MET	C-N-CA	5.63	135.77	121.70
1	A	195	LEU	N-CA-C	-5.61	95.86	111.00
1	B	61	GLU	C-N-CA	5.61	135.71	121.70
1	C	36	GLY	N-CA-C	-5.60	99.10	113.10
1	C	180	PRO	C-N-CA	5.59	135.68	121.70
1	A	222	THR	N-CA-C	5.53	125.92	111.00
1	C	122	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	59	MET	N-CA-C	5.51	125.88	111.00
1	A	180	PRO	C-N-CA	5.46	135.34	121.70
1	B	180	PRO	C-N-CA	5.45	135.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	218	PRO	CA-C-N	5.43	127.07	116.20
1	B	165	VAL	CB-CA-C	5.43	121.72	111.40
1	A	221	TYR	C-N-CA	5.42	135.26	121.70
1	B	165	VAL	C-N-CA	5.42	135.25	121.70
1	C	237	HIS	N-CA-C	5.39	125.56	111.00
1	C	62	TYR	N-CA-CB	5.33	120.19	110.60
1	B	235	MET	C-N-CA	5.29	134.91	121.70
1	C	233	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	76	ALA	N-CA-C	-5.25	96.82	111.00
1	A	36	GLY	N-CA-C	-5.25	99.97	113.10
1	A	51	VAL	N-CA-C	-5.24	96.85	111.00
1	A	237	HIS	N-CA-C	5.23	125.12	111.00
1	C	233	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	C	51	VAL	CA-C-N	5.17	128.58	117.20
1	B	73	ASP	N-CA-CB	5.15	119.86	110.60
1	C	235	MET	CA-C-N	-5.15	105.88	117.20
1	C	236	LYS	CA-CB-CG	5.13	124.70	113.40
1	C	236	LYS	N-CA-CB	5.09	119.76	110.60
1	C	212	CYS	CA-CB-SG	5.01	123.01	114.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	53	THR	CA
1	C	216	ASN	CA
1	C	236	LYS	CA

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	LYS	Peptide
1	A	199	GLY	Peptide
1	A	212	CYS	Peptide
1	A	214	GLN	Peptide
1	A	221	TYR	Peptide
1	A	58	LYS	Peptide
1	A	59	MET	Peptide
1	A	60	ASN	Peptide
1	A	61	GLU	Peptide
1	A	73	ASP	Peptide
1	B	165	VAL	Peptide
1	B	183	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	212	CYS	Mainchain,Peptide
1	B	214	GLN	Peptide
1	B	218	PRO	Peptide
1	B	235	MET	Peptide
1	B	61	GLU	Peptide
1	B	72	GLY	Peptide
1	C	165	VAL	Peptide
1	C	166	TYR	Peptide
1	C	183	LYS	Peptide
1	C	195	LEU	Peptide
1	C	199	GLY	Peptide
1	C	211	PRO	Peptide
1	C	212	CYS	Peptide
1	C	214	GLN	Peptide
1	C	220	VAL	Peptide
1	C	237	HIS	Peptide
1	C	52	LEU	Peptide
1	C	60	ASN	Peptide
1	C	61	GLU	Peptide
1	C	76	ALA	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	1679	0	1638	127	0
1	B	1664	0	1641	124	0
1	C	1695	0	1673	124	0
2	A	30	0	0	1	0
2	B	30	0	0	5	0
2	C	20	0	0	0	0
3	A	16	0	0	5	0
3	B	6	0	0	2	0
3	C	8	0	0	1	0
All	All	5148	0	4952	364	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 36.

All (364) 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:214:GLN:CG	1:C:215:PRO:HD3	1.35	1.51
1:C:182:SER:HB3	1:C:183:LYS:CB	1.53	1.38
1:A:182:SER:HB3	1:A:183:LYS:CB	1.54	1.36
1:C:214:GLN:HB2	1:C:215:PRO:CG	1.56	1.35
1:B:182:SER:HB3	1:B:183:LYS:CB	1.59	1.30
1:C:187:CYS:CB	1:C:212:CYS:SG	2.21	1.28
1:C:214:GLN:HG3	1:C:215:PRO:CD	1.65	1.24
1:B:65:HIS:CD2	1:C:122:ARG:HH12	1.56	1.23
1:B:180:PRO:CB	1:B:181:ASP:HB2	1.67	1.23
1:A:214:GLN:HG2	1:A:215:PRO:CD	1.68	1.22
1:A:180:PRO:CB	1:A:181:ASP:HB2	1.71	1.20
1:B:180:PRO:O	1:B:216:ASN:OD1	1.61	1.18
1:B:182:SER:HB3	1:B:183:LYS:CA	1.71	1.17
1:C:182:SER:HB3	1:C:183:LYS:CA	1.74	1.17
1:A:182:SER:HB3	1:A:183:LYS:CA	1.74	1.16
1:A:142:ASP:OD2	1:B:168:ASP:HB2	1.46	1.15
1:C:180:PRO:CB	1:C:181:ASP:HB2	1.78	1.14
1:A:236:LYS:CE	1:A:236:LYS:H	1.60	1.14
1:B:236:LYS:H	1:B:236:LYS:CE	1.60	1.14
1:A:109:ARG:HH11	1:A:109:ARG:CG	1.59	1.12
1:B:214:GLN:CB	1:B:215:PRO:HD2	1.77	1.12
1:C:214:GLN:CB	1:C:215:PRO:HD3	1.74	1.10
1:A:214:GLN:CB	1:A:215:PRO:CD	2.30	1.10
1:B:214:GLN:CB	1:B:215:PRO:CD	2.30	1.10
1:B:182:SER:HB3	1:B:183:LYS:HB2	1.18	1.09
1:A:214:GLN:CG	1:A:215:PRO:CD	2.30	1.08
1:A:236:LYS:HA	1:A:237:HIS:O	1.53	1.08
1:A:180:PRO:HB2	1:A:181:ASP:CB	1.84	1.08
1:B:62:TYR:HB2	1:B:81:ALA:HB3	1.36	1.07
1:C:214:GLN:CB	1:C:215:PRO:CD	2.29	1.07
1:C:183:LYS:N	1:C:184:LYS:HB2	1.70	1.05
1:C:182:SER:HB3	1:C:183:LYS:HB2	1.11	1.05
1:A:182:SER:HB3	1:A:183:LYS:HB2	1.13	1.05
1:A:214:GLN:HG2	1:A:215:PRO:HD2	1.31	1.05
1:A:236:LYS:H	1:A:236:LYS:HE3	1.22	1.05
1:C:62:TYR:HB2	1:C:81:ALA:HB3	1.38	1.05
1:B:180:PRO:HB2	1:B:181:ASP:CB	1.85	1.04
1:C:180:PRO:HB2	1:C:181:ASP:CB	1.87	1.03
1:A:109:ARG:HH11	1:A:109:ARG:HG3	0.87	1.02
1:A:214:GLN:CG	1:A:215:PRO:HD2	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLY:HA2	1:A:68:SER:HB2	1.42	1.01
1:B:236:LYS:H	1:B:236:LYS:HE3	1.25	1.01
1:B:214:GLN:HB2	1:B:215:PRO:HD2	1.38	1.00
1:B:236:LYS:H	1:B:236:LYS:NZ	1.59	1.00
1:C:214:GLN:HB2	1:C:215:PRO:CD	1.88	1.00
1:C:67:GLY:CA	1:C:68:SER:HB2	1.92	0.99
1:C:124:GLU:HG3	1:C:128:THR:HG21	1.45	0.99
1:A:124:GLU:HG3	1:A:128:THR:HG21	1.44	0.99
1:B:199:GLY:HA3	1:B:200:THR:HB	1.45	0.99
1:A:214:GLN:CG	1:A:215:PRO:HD3	1.90	0.99
1:B:65:HIS:HD2	1:C:122:ARG:NH1	1.59	0.98
1:A:76:ALA:HB1	1:A:77:GLN:HA	1.44	0.98
1:C:182:SER:CB	1:C:183:LYS:HB2	1.93	0.97
1:C:236:LYS:O	1:C:236:LYS:HE2	1.64	0.97
1:A:183:LYS:O	1:A:183:LYS:HG2	1.62	0.97
1:B:182:SER:CB	1:B:183:LYS:HA	1.94	0.96
1:A:62:TYR:HB2	1:A:81:ALA:HB3	1.46	0.96
1:C:183:LYS:O	1:C:183:LYS:HG2	1.62	0.96
1:C:214:GLN:HB2	1:C:215:PRO:HG3	0.98	0.96
1:A:168:ASP:HB2	1:B:142:ASP:OD2	1.66	0.95
1:B:67:GLY:HA2	1:B:68:SER:HB2	1.45	0.95
1:C:214:GLN:CB	1:C:215:PRO:HG3	1.95	0.95
1:B:124:GLU:HG3	1:B:128:THR:HG21	1.46	0.95
1:C:214:GLN:CB	1:C:215:PRO:CG	2.45	0.95
1:A:67:GLY:CA	1:A:68:SER:HB2	1.96	0.95
1:C:67:GLY:HA2	1:C:68:SER:HB2	1.47	0.95
1:A:182:SER:CB	1:A:183:LYS:HB2	1.96	0.95
1:C:214:GLN:CG	1:C:215:PRO:CD	2.30	0.94
1:B:183:LYS:N	1:B:184:LYS:HB2	1.81	0.94
1:C:182:SER:CB	1:C:183:LYS:CA	2.44	0.93
1:B:183:LYS:HG2	1:B:183:LYS:O	1.67	0.93
1:A:236:LYS:H	1:A:236:LYS:NZ	1.64	0.93
1:B:67:GLY:CA	1:B:68:SER:HB2	1.98	0.92
1:A:182:SER:HB2	1:A:215:PRO:HA	1.49	0.92
1:A:214:GLN:CB	1:A:215:PRO:HD2	1.98	0.91
1:B:76:ALA:HB1	1:B:77:GLN:HA	1.51	0.91
1:C:182:SER:CB	1:C:183:LYS:HA	1.98	0.91
1:A:182:SER:CB	1:A:183:LYS:CA	2.47	0.91
1:A:109:ARG:HG3	1:A:109:ARG:NH1	1.61	0.91
1:C:212:CYS:SG	1:C:212:CYS:O	2.29	0.90
1:B:182:SER:CB	1:B:183:LYS:HB2	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ALA:HB1	1:C:77:GLN:HA	1.53	0.90
1:C:180:PRO:HB2	1:C:181:ASP:HB2	0.92	0.90
1:A:199:GLY:HA3	1:A:200:THR:HB	1.55	0.89
1:A:182:SER:CB	1:A:183:LYS:HA	2.02	0.88
1:A:183:LYS:N	1:A:184:LYS:HB2	1.89	0.88
1:C:183:LYS:HZ3	1:C:214:GLN:HE21	1.19	0.88
1:B:180:PRO:HB2	1:B:181:ASP:HB2	0.92	0.88
1:A:122:ARG:HD3	3:A:249:HOH:O	1.72	0.88
1:A:180:PRO:HB2	1:A:181:ASP:HB2	0.89	0.87
1:B:182:SER:CB	1:B:183:LYS:CA	2.43	0.86
1:C:67:GLY:HA2	1:C:68:SER:CB	2.04	0.86
1:A:214:GLN:HG2	1:A:215:PRO:HD3	1.52	0.85
1:B:236:LYS:NZ	1:B:236:LYS:N	2.24	0.85
1:C:187:CYS:HG	1:C:212:CYS:CB	1.88	0.85
1:B:182:SER:HB3	1:B:183:LYS:HA	1.56	0.84
1:A:236:LYS:NZ	1:A:236:LYS:N	2.24	0.84
1:B:214:GLN:HB3	1:B:215:PRO:HD2	1.56	0.84
1:B:236:LYS:HA	1:B:237:HIS:C	1.98	0.83
1:A:67:GLY:HA2	1:A:68:SER:CB	2.05	0.83
1:B:67:GLY:HA2	1:B:68:SER:CB	2.08	0.82
1:C:215:PRO:O	1:C:216:ASN:HB3	1.77	0.82
1:C:236:LYS:HA	1:C:237:HIS:O	1.80	0.81
1:B:65:HIS:CD2	1:C:122:ARG:NH1	2.41	0.80
1:A:237:HIS:HA	1:A:238:HIS:C	2.02	0.80
1:C:180:PRO:O	1:C:216:ASN:OD1	2.00	0.80
1:C:214:GLN:HG3	1:C:215:PRO:HD3	0.81	0.79
1:A:182:SER:CB	1:A:215:PRO:HA	2.12	0.79
1:C:183:LYS:O	1:C:183:LYS:CG	2.30	0.79
1:A:236:LYS:HE3	1:A:236:LYS:N	1.98	0.78
1:B:42:GLY:O	1:B:53:THR:HG23	1.83	0.78
1:C:236:LYS:HA	1:C:237:HIS:C	2.03	0.78
1:B:214:GLN:HB3	1:B:215:PRO:CD	2.11	0.78
1:B:125:PRO:O	1:B:128:THR:HG22	1.84	0.78
1:B:236:LYS:HE3	1:B:236:LYS:N	1.98	0.77
1:A:183:LYS:O	1:A:183:LYS:CG	2.33	0.77
1:B:183:LYS:O	1:B:183:LYS:CG	2.33	0.76
1:A:191:SER:HA	1:A:205:VAL:HG22	1.66	0.76
1:B:214:GLN:HB2	1:B:215:PRO:CD	2.06	0.76
1:A:62:TYR:HB2	1:A:81:ALA:CB	2.15	0.75
1:A:125:PRO:O	1:A:128:THR:HG22	1.88	0.74
1:B:65:HIS:HD2	1:C:122:ARG:HH12	0.82	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ASP:O	1:C:236:LYS:NZ	2.19	0.74
1:B:76:ALA:CB	1:B:77:GLN:HA	2.18	0.73
1:C:125:PRO:O	1:C:128:THR:HG22	1.88	0.73
1:A:214:GLN:HB3	1:A:215:PRO:HD2	1.69	0.72
1:B:78:ARG:HD3	3:B:241:HOH:O	1.89	0.72
1:C:215:PRO:O	1:C:216:ASN:CB	2.37	0.72
1:C:182:SER:HB3	1:C:183:LYS:HA	1.62	0.72
1:C:183:LYS:NZ	1:C:214:GLN:HE21	1.87	0.72
1:A:236:LYS:N	1:A:236:LYS:HZ1	1.87	0.71
1:A:142:ASP:OD2	1:B:168:ASP:CB	2.34	0.70
1:A:51:VAL:O	1:A:102:VAL:N	2.20	0.70
1:B:180:PRO:C	1:B:216:ASN:OD1	2.30	0.69
1:A:91:SER:O	1:A:92:THR:HB	1.91	0.69
1:A:42:GLY:O	1:A:53:THR:HG23	1.91	0.69
1:C:62:TYR:HB2	1:C:81:ALA:CB	2.21	0.69
1:C:154:VAL:HG13	1:C:177:ALA:HB1	1.74	0.69
1:C:183:LYS:HZ3	1:C:214:GLN:NE2	1.89	0.69
1:A:109:ARG:N	1:A:109:ARG:CD	2.57	0.68
1:A:141:PRO:HB2	1:B:169:LEU:HD11	1.75	0.68
1:B:139:THR:OG1	1:B:144:THR:OG1	2.10	0.68
1:A:109:ARG:CG	1:A:109:ARG:NH1	2.33	0.68
1:C:187:CYS:CA	1:C:212:CYS:SG	2.81	0.68
1:B:62:TYR:HB2	1:B:81:ALA:CB	2.20	0.68
1:A:182:SER:CB	1:A:183:LYS:CB	2.51	0.68
1:A:233:ASP:O	1:A:236:LYS:NZ	2.26	0.67
1:C:191:SER:HA	1:C:205:VAL:HG22	1.75	0.67
1:B:233:ASP:O	1:B:236:LYS:NZ	2.27	0.67
1:C:154:VAL:CG1	1:C:177:ALA:HB1	2.24	0.66
1:B:175:LEU:O	1:B:221:TYR:HB2	1.95	0.66
1:B:191:SER:HA	1:B:205:VAL:HG22	1.76	0.66
1:A:60:ASN:HD22	1:A:61:GLU:H	1.44	0.66
1:C:197:CYS:O	1:C:200:THR:HG22	1.96	0.66
1:A:154:VAL:HG13	1:A:177:ALA:HB1	1.79	0.65
1:A:175:LEU:O	1:A:221:TYR:HB2	1.96	0.65
1:B:125:PRO:O	1:B:128:THR:CG2	2.45	0.65
1:B:61:GLU:HA	1:B:62:TYR:CD1	2.32	0.64
1:A:125:PRO:O	1:A:128:THR:CG2	2.45	0.64
1:C:51:VAL:O	1:C:102:VAL:N	2.21	0.64
1:A:154:VAL:CG1	1:A:177:ALA:HB1	2.28	0.64
1:B:199:GLY:HA3	1:B:200:THR:CB	2.25	0.64
1:C:129:THR:OG1	1:C:155:LYS:HE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:HB1	1:A:77:GLN:CA	2.25	0.64
1:A:214:GLN:HB3	1:A:215:PRO:CD	2.25	0.63
1:B:236:LYS:CE	1:B:236:LYS:N	2.46	0.63
1:B:236:LYS:CA	1:B:237:HIS:C	2.67	0.63
1:C:183:LYS:CA	1:C:184:LYS:HB2	2.29	0.62
1:B:62:TYR:CB	1:B:81:ALA:HB3	2.22	0.62
1:A:236:LYS:CE	1:A:236:LYS:N	2.46	0.62
1:A:60:ASN:HD22	1:A:61:GLU:N	1.98	0.61
1:A:76:ALA:CB	1:A:77:GLN:HA	2.24	0.61
1:C:42:GLY:O	1:C:53:THR:HG23	2.00	0.61
1:B:154:VAL:HG13	1:B:177:ALA:HB1	1.83	0.61
1:B:236:LYS:N	1:B:236:LYS:HZ1	1.95	0.61
1:A:183:LYS:CA	1:A:184:LYS:HB2	2.30	0.61
1:B:183:LYS:CA	1:B:184:LYS:HB2	2.30	0.60
1:C:182:SER:C	1:C:184:LYS:HB2	2.19	0.60
1:B:182:SER:HB2	1:B:215:PRO:HA	1.82	0.60
1:B:236:LYS:NZ	1:B:236:LYS:O	2.28	0.60
1:A:103:LYS:HZ1	1:A:238:HIS:H	1.50	0.60
1:C:62:TYR:CB	1:C:81:ALA:HB3	2.23	0.60
1:A:160:GLN:O	1:A:163:THR:HG22	2.01	0.60
1:C:125:PRO:O	1:C:128:THR:CG2	2.50	0.60
1:A:58:LYS:HA	1:A:62:TYR:OH	2.02	0.60
1:C:67:GLY:CA	1:C:68:SER:CB	2.67	0.59
1:B:76:ALA:CB	1:B:77:GLN:CA	2.81	0.59
1:A:159:PRO:O	1:A:163:THR:HB	2.02	0.59
1:A:75:ARG:HA	1:A:76:ALA:HB2	1.83	0.59
1:A:141:PRO:HB2	1:B:169:LEU:CD1	2.33	0.59
1:B:214:GLN:CB	1:B:215:PRO:HD3	2.32	0.58
1:C:175:LEU:HB2	1:C:223:GLN:HG3	1.85	0.58
1:C:182:SER:OG	1:C:215:PRO:HA	2.03	0.58
1:B:182:SER:OG	1:B:183:LYS:HA	2.02	0.58
1:B:216:ASN:N	3:B:239:HOH:O	2.18	0.58
1:B:197:CYS:O	1:B:200:THR:HG22	2.03	0.58
1:C:182:SER:OG	1:C:183:LYS:HA	2.04	0.58
1:C:128:THR:HG23	1:C:156:LEU:HD12	1.86	0.58
1:C:209:THR:O	1:C:212:CYS:HA	2.03	0.58
1:A:236:LYS:NZ	1:A:236:LYS:O	2.27	0.58
1:A:34:LEU:HD23	1:A:39:LEU:HA	1.86	0.58
1:B:106:SER:HA	2:B:12:SO4:O4	2.04	0.58
1:A:154:VAL:HG22	1:A:178:GLY:HA2	1.86	0.57
1:C:76:ALA:HB1	1:C:77:GLN:CA	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLY:HA2	1:A:222:THR:O	2.03	0.57
1:C:183:LYS:NZ	1:C:214:GLN:NE2	2.49	0.57
1:A:103:LYS:NZ	1:A:238:HIS:N	2.52	0.57
1:A:236:LYS:HA	1:A:237:HIS:C	2.22	0.57
1:A:175:LEU:HB2	1:A:223:GLN:HG3	1.87	0.56
1:C:91:SER:O	1:C:92:THR:HB	2.03	0.56
1:C:204:LEU:O	1:C:221:TYR:HA	2.05	0.56
1:B:154:VAL:CG1	1:B:177:ALA:HB1	2.37	0.55
1:A:197:CYS:O	1:A:200:THR:HG22	2.07	0.55
1:B:181:ASP:N	1:B:216:ASN:OD1	2.40	0.55
1:B:182:SER:C	1:B:184:LYS:HB2	2.26	0.55
1:A:81:ALA:O	1:A:82:SER:HB2	2.05	0.55
1:B:34:LEU:HD23	1:B:39:LEU:HA	1.88	0.55
1:C:139:THR:OG1	1:C:144:THR:OG1	2.26	0.54
1:C:34:LEU:HD23	1:C:39:LEU:HA	1.89	0.54
1:A:109:ARG:N	1:A:109:ARG:HD3	2.23	0.54
1:A:185:ASN:N	1:A:185:ASN:HD22	2.04	0.54
1:C:66:LEU:O	1:C:77:GLN:N	2.23	0.54
1:A:91:SER:O	1:A:92:THR:CB	2.56	0.54
1:A:199:GLY:HA3	1:A:200:THR:CB	2.35	0.53
1:C:137:THR:CG2	1:C:187:CYS:SG	2.96	0.53
1:B:175:LEU:HB2	1:B:223:GLN:HG3	1.90	0.53
1:B:51:VAL:O	1:B:102:VAL:N	2.21	0.53
1:C:228:THR:O	1:C:232:ASN:ND2	2.41	0.53
1:C:61:GLU:HA	1:C:62:TYR:CD1	2.44	0.53
1:A:16:ILE:N	3:A:247:HOH:O	2.41	0.53
1:C:156:LEU:HD22	1:C:175:LEU:HD11	1.91	0.53
1:C:160:GLN:O	1:C:163:THR:HG22	2.09	0.53
1:C:183:LYS:HG3	1:C:214:GLN:CB	2.39	0.53
1:C:76:ALA:CB	1:C:77:GLN:HA	2.32	0.52
1:B:176:CYS:HA	1:B:219:GLY:O	2.10	0.52
1:B:46:VAL:O	1:B:116:LYS:HG2	2.10	0.52
1:B:215:PRO:O	1:B:216:ASN:HB2	2.10	0.52
1:A:197:CYS:O	1:A:198:ARG:C	2.47	0.51
1:B:128:THR:HG23	1:B:156:LEU:HD12	1.91	0.51
1:B:236:LYS:HZ2	1:B:236:LYS:C	2.11	0.51
1:C:236:LYS:O	1:C:236:LYS:CE	2.50	0.51
1:A:182:SER:C	1:A:184:LYS:HB2	2.30	0.51
1:A:204:LEU:O	1:A:221:TYR:HA	2.11	0.51
1:B:81:ALA:O	1:B:82:SER:HB2	2.10	0.51
1:C:49:ARG:NH2	3:C:240:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:CYS:HA	1:C:212:CYS:SG	2.49	0.51
1:A:103:LYS:NZ	1:A:238:HIS:H	2.06	0.51
1:B:160:GLN:O	1:B:163:THR:HG22	2.10	0.51
1:C:182:SER:CB	1:C:215:PRO:HA	2.41	0.51
1:A:76:ALA:CB	1:A:77:GLN:CA	2.85	0.51
1:B:81:ALA:O	1:B:105:ASN:OD1	2.28	0.50
1:B:154:VAL:HG22	1:B:178:GLY:HA2	1.93	0.50
1:C:75:ARG:HG3	1:C:76:ALA:HB2	1.94	0.50
1:C:183:LYS:HG3	1:C:214:GLN:HB3	1.92	0.50
1:B:159:PRO:O	1:B:163:THR:HB	2.12	0.50
1:B:137:THR:CG2	1:B:187:CYS:SG	2.99	0.50
1:C:203:GLY:HA2	1:C:222:THR:O	2.12	0.50
1:B:73:ASP:O	1:B:74:ARG:C	2.50	0.49
1:A:46:VAL:O	1:A:116:LYS:HG2	2.12	0.49
1:C:46:VAL:O	1:C:116:LYS:HG2	2.13	0.49
1:A:185:ASN:N	1:A:185:ASN:ND2	2.61	0.49
1:C:76:ALA:CB	1:C:77:GLN:CA	2.91	0.49
1:C:185:ASN:N	1:C:185:ASN:HD22	2.10	0.48
1:B:47:ASN:HA	1:B:116:LYS:CG	2.44	0.48
1:B:164:LYS:HE2	1:B:164:LYS:HA	1.95	0.48
1:B:197:CYS:O	1:B:198:ARG:C	2.51	0.48
1:A:236:LYS:CA	1:A:237:HIS:O	2.44	0.48
1:C:163:THR:O	1:C:167:LYS:HA	2.13	0.48
1:A:183:LYS:HG3	1:A:214:GLN:HG3	1.95	0.48
1:B:26:SER:OG	1:B:27:HIS:HD2	1.97	0.48
1:B:214:GLN:HB3	1:B:215:PRO:HD3	1.92	0.47
1:C:235:MET:O	1:C:236:LYS:NZ	2.46	0.47
1:A:74:ARG:H	1:A:75:ARG:C	2.17	0.47
1:A:187:CYS:SG	1:A:188:ASN:N	2.87	0.47
1:B:58:LYS:NZ	2:B:2:SO4:O2	2.44	0.47
1:B:228:THR:O	1:B:232:ASN:ND2	2.48	0.47
1:B:52:LEU:HD22	1:B:52:LEU:HA	1.71	0.47
1:A:60:ASN:H	1:A:61:GLU:CA	2.26	0.47
1:A:60:ASN:H	1:A:61:GLU:HA	1.79	0.47
1:C:175:LEU:HB2	1:C:223:GLN:CG	2.44	0.47
1:A:182:SER:OG	1:A:183:LYS:HA	2.15	0.47
1:B:62:TYR:CB	1:B:81:ALA:CB	2.89	0.46
1:B:91:SER:O	1:B:92:THR:HB	2.16	0.46
1:B:131:THR:O	1:B:195:LEU:HA	2.15	0.46
1:C:197:CYS:O	1:C:198:ARG:C	2.53	0.46
1:C:70:THR:HA	1:C:147:SER:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:MET:C	1:C:236:LYS:HZ2	2.19	0.46
1:A:175:LEU:O	1:A:220:VAL:HA	2.16	0.46
1:C:91:SER:O	1:C:92:THR:CB	2.64	0.46
1:C:154:VAL:HG22	1:C:178:GLY:HA2	1.98	0.46
1:C:26:SER:OG	1:C:27:HIS:HD2	1.99	0.45
1:C:32:ALA:HB3	1:C:65:HIS:HB3	1.98	0.45
1:C:185:ASN:N	1:C:185:ASN:ND2	2.65	0.45
1:C:70:THR:O	1:C:72:GLY:HA2	2.16	0.45
1:A:129:THR:OG1	1:A:155:LYS:HE2	2.16	0.45
1:A:185:ASN:CB	3:A:250:HOH:O	2.64	0.45
1:B:137:THR:HG23	1:B:187:CYS:SG	2.57	0.45
1:B:90:TYR:HA	1:B:96:VAL:O	2.17	0.45
1:A:29:TRP:HB2	1:A:117:VAL:HG13	1.99	0.45
1:C:29:TRP:HB2	1:C:117:VAL:HG13	1.99	0.45
1:A:47:ASN:HA	1:A:116:LYS:CG	2.47	0.44
1:A:86:ARG:HB2	2:A:1:SO4:O4	2.17	0.44
1:A:228:THR:O	1:A:232:ASN:ND2	2.50	0.44
1:A:141:PRO:O	1:B:169:LEU:HD11	2.18	0.44
1:A:128:THR:HG23	1:A:156:LEU:HD12	2.00	0.44
1:B:129:THR:OG1	1:B:155:LYS:HE2	2.18	0.44
1:A:108:ALA:C	1:A:109:ARG:CD	2.85	0.44
1:B:182:SER:CB	1:B:215:PRO:HA	2.47	0.44
1:A:75:ARG:CA	1:A:76:ALA:HB2	2.48	0.44
1:B:95:HIS:CD2	2:B:14:SO4:S	3.11	0.44
1:B:203:GLY:HA2	1:B:222:THR:O	2.17	0.44
1:A:32:ALA:HB3	1:A:65:HIS:HB3	2.00	0.44
1:C:45:LEU:O	1:C:117:VAL:HG22	2.17	0.44
1:C:159:PRO:O	1:C:163:THR:HB	2.18	0.44
1:B:32:ALA:HB3	1:B:65:HIS:HB3	1.99	0.43
1:B:95:HIS:HD2	2:B:14:SO4:O2	2.01	0.43
1:B:175:LEU:O	1:B:220:VAL:HA	2.18	0.43
1:B:223:GLN:HE22	1:B:226:LYS:NZ	2.15	0.43
1:C:62:TYR:CB	1:C:81:ALA:CB	2.90	0.43
1:C:129:THR:HA	1:C:155:LYS:HD3	2.00	0.43
1:A:185:ASN:HB3	3:A:250:HOH:O	2.18	0.43
1:C:31:VAL:HG12	1:C:66:LEU:HB3	2.00	0.43
1:C:47:ASN:HA	1:C:116:LYS:CG	2.49	0.43
1:B:31:VAL:HG12	1:B:66:LEU:HB3	2.00	0.43
1:A:53:THR:HG22	1:A:54:ALA:H	1.83	0.43
1:A:108:ALA:C	1:A:109:ARG:HD3	2.38	0.43
1:A:199:GLY:CA	1:A:200:THR:HB	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:O	1:A:117:VAL:HG22	2.19	0.43
1:A:103:LYS:HZ3	1:A:238:HIS:N	2.16	0.43
1:A:169:LEU:HD11	1:B:141:PRO:O	2.19	0.43
1:B:236:LYS:N	1:B:236:LYS:HZ2	2.13	0.43
1:C:211:PRO:O	1:C:213:GLY:HA2	2.18	0.43
1:C:37:ASN:HD22	1:C:37:ASN:HA	1.67	0.43
1:B:199:GLY:CA	1:B:200:THR:HB	2.30	0.42
1:C:73:ASP:O	1:C:74:ARG:C	2.58	0.42
1:C:216:ASN:HD22	1:C:216:ASN:HA	1.47	0.42
1:C:90:TYR:HA	1:C:96:VAL:O	2.20	0.42
1:C:235:MET:C	1:C:236:LYS:NZ	2.72	0.42
1:A:96:VAL:HG13	1:A:171:GLU:HG3	2.01	0.42
1:A:81:ALA:O	1:A:82:SER:CB	2.67	0.42
1:B:204:LEU:O	1:B:221:TYR:HA	2.20	0.42
1:C:223:GLN:HE22	1:C:226:LYS:NZ	2.17	0.42
1:C:55:ALA:HB1	1:C:86:ARG:CG	2.49	0.42
1:C:232:ASN:HA	1:C:235:MET:HG3	2.02	0.42
1:B:47:ASN:HA	1:B:116:LYS:HG3	2.02	0.41
1:B:95:HIS:CD2	2:B:14:SO4:O2	2.73	0.41
1:A:193:GLY:HA3	3:A:251:HOH:O	2.20	0.41
1:A:236:LYS:HZ2	1:A:236:LYS:C	2.16	0.41
1:A:52:LEU:HD22	1:A:52:LEU:HA	1.63	0.41
1:B:53:THR:HG22	1:B:54:ALA:H	1.85	0.41
1:C:73:ASP:O	1:C:75:ARG:N	2.53	0.41
1:C:211:PRO:O	1:C:213:GLY:CA	2.69	0.41
1:A:217:ASP:HA	1:A:218:PRO:HD3	1.68	0.41
1:C:31:VAL:CG1	1:C:66:LEU:HD23	2.50	0.41
1:B:180:PRO:CA	1:B:181:ASP:HB2	2.44	0.41
1:B:236:LYS:HA	1:B:237:HIS:O	2.17	0.41
1:C:81:ALA:O	1:C:82:SER:HB2	2.21	0.41
1:A:103:LYS:HZ1	1:A:238:HIS:N	2.12	0.40
1:B:175:LEU:HB2	1:B:223:GLN:CG	2.52	0.40
1:C:132:VAL:HB	1:C:195:LEU:HD23	2.02	0.40
1:B:87:HIS:ND1	1:B:97:ASN:HB3	2.36	0.40
1:B:163:THR:HA	1:B:170:LEU:HD12	2.03	0.40
1:B:179:ILE:O	1:B:182:SER:N	2.50	0.40
1:B:29:TRP:HB2	1:B:117:VAL:HG13	2.04	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	221/227 (97%)	182 (82%)	22 (10%)	17 (8%)	1	2
1	B	217/227 (96%)	180 (83%)	17 (8%)	20 (9%)	1	1
1	C	221/227 (97%)	180 (81%)	25 (11%)	16 (7%)	1	2
All	All	659/681 (97%)	542 (82%)	64 (10%)	53 (8%)	1	2

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	167	LYS
1	A	180	PRO
1	A	184	LYS
1	A	200	THR
1	A	237	HIS
1	B	62	TYR
1	B	68	SER
1	B	166	TYR
1	B	167	LYS
1	B	180	PRO
1	B	184	LYS
1	B	200	THR
1	B	221	TYR
1	C	62	TYR
1	C	68	SER
1	C	180	PRO
1	C	184	LYS
1	C	214	GLN
1	C	237	HIS
1	A	76	ALA
1	A	92	THR
1	A	181	ASP
1	A	195	LEU

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Mol	Chain	Res	Type
1	A	196	VAL
1	A	198	ARG
1	A	222	THR
1	A	225	CYS
1	B	76	ALA
1	B	92	THR
1	B	181	ASP
1	B	196	VAL
1	C	53	THR
1	C	92	THR
1	C	181	ASP
1	A	52	LEU
1	A	60	ASN
1	A	221	TYR
1	B	74	ARG
1	B	225	CYS
1	C	182	SER
1	C	236	LYS
1	B	52	LEU
1	B	185	ASN
1	B	198	ARG
1	B	219	GLY
1	B	61	GLU
1	B	182	SER
1	C	74	ARG
1	C	185	ASN
1	C	198	ARG
1	C	225	CYS
1	C	215	PRO

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	190/197 (96%)	154 (81%)	36 (19%)	1 5
1	B	189/197 (96%)	152 (80%)	37 (20%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	193/197 (98%)	155 (80%)	38 (20%)	1 4
All	All	572/591 (97%)	461 (81%)	111 (19%)	1 4

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	44	VAL
1	A	52	LEU
1	A	53	THR
1	A	60	ASN
1	A	66	LEU
1	A	68	SER
1	A	83	LYS
1	A	86	ARG
1	A	92	THR
1	A	94	THR
1	A	109	ARG
1	A	117	VAL
1	A	121	SER
1	A	122	ARG
1	A	128	THR
1	A	139	THR
1	A	143	VAL
1	A	144	THR
1	A	151	CYS
1	A	154	VAL
1	A	160	GLN
1	A	163	THR
1	A	182	SER
1	A	183	LYS
1	A	184	LYS
1	A	185	ASN
1	A	198	ARG
1	A	200	THR
1	A	205	VAL
1	A	215	PRO
1	A	222	THR
1	A	232	ASN
1	A	235	MET
1	A	236	LYS
1	A	238	HIS

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Mol	Chain	Res	Type
1	B	22	CYS
1	B	30	GLN
1	B	37	ASN
1	B	44	VAL
1	B	52	LEU
1	B	53	THR
1	B	60	ASN
1	B	66	LEU
1	B	78	ARG
1	B	83	LYS
1	B	86	ARG
1	B	92	THR
1	B	94	THR
1	B	109	ARG
1	B	117	VAL
1	B	121	SER
1	B	128	THR
1	B	130	CYS
1	B	139	THR
1	B	143	VAL
1	B	144	THR
1	B	151	CYS
1	B	154	VAL
1	B	160	GLN
1	B	180	PRO
1	B	182	SER
1	B	183	LYS
1	B	184	LYS
1	B	185	ASN
1	B	198	ARG
1	B	200	THR
1	B	205	VAL
1	B	214	GLN
1	B	226	LYS
1	B	232	ASN
1	B	235	MET
1	B	236	LYS
1	C	22	CYS
1	C	30	GLN
1	C	44	VAL
1	C	52	LEU
1	C	53	THR

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Mol	Chain	Res	Type
1	C	60	ASN
1	C	66	LEU
1	C	68	SER
1	C	74	ARG
1	C	77	GLN
1	C	78	ARG
1	C	83	LYS
1	C	86	ARG
1	C	92	THR
1	C	94	THR
1	C	117	VAL
1	C	121	SER
1	C	122	ARG
1	C	128	THR
1	C	139	THR
1	C	143	VAL
1	C	144	THR
1	C	151	CYS
1	C	154	VAL
1	C	160	GLN
1	C	182	SER
1	C	183	LYS
1	C	184	LYS
1	C	185	ASN
1	C	198	ARG
1	C	200	THR
1	C	205	VAL
1	C	212	CYS
1	C	214	GLN
1	C	216	ASN
1	C	232	ASN
1	C	235	MET
1	C	236	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	30	GLN
1	A	37	ASN
1	A	60	ASN
1	A	65	HIS

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Mol	Chain	Res	Type
1	A	77	GLN
1	A	107	GLN
1	A	185	ASN
1	A	188	ASN
1	A	223	GLN
1	A	232	ASN
1	B	27	HIS
1	B	30	GLN
1	B	37	ASN
1	B	38	GLN
1	B	60	ASN
1	B	65	HIS
1	B	77	GLN
1	B	95	HIS
1	B	107	GLN
1	B	185	ASN
1	B	188	ASN
1	B	223	GLN
1	B	232	ASN
1	C	27	HIS
1	C	30	GLN
1	C	37	ASN
1	C	60	ASN
1	C	77	GLN
1	C	107	GLN
1	C	185	ASN
1	C	188	ASN
1	C	214	GLN
1	C	216	ASN
1	C	223	GLN
1	C	232	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
2	SO4	A	8	-	4,4,4	0.13	0	6,6,6	0.41	0
2	SO4	A	1	-	4,4,4	0.17	0	6,6,6	0.54	0
2	SO4	C	6	-	4,4,4	0.17	0	6,6,6	0.26	0
2	SO4	B	10	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	A	7	-	4,4,4	0.21	0	6,6,6	0.46	0
2	SO4	C	239	-	4,4,4	0.10	0	6,6,6	0.35	0
2	SO4	C	4	-	4,4,4	0.16	0	6,6,6	0.72	0
2	SO4	B	15	-	4,4,4	0.12	0	6,6,6	0.20	0
2	SO4	B	2	-	4,4,4	0.16	0	6,6,6	0.93	0
2	SO4	C	3	-	4,4,4	0.15	0	6,6,6	0.36	0
2	SO4	B	14	-	4,4,4	0.12	0	6,6,6	0.26	0
2	SO4	A	5	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	B	12	-	4,4,4	0.21	0	6,6,6	0.49	0
2	SO4	B	11	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	A	13	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	A	9	-	4,4,4	0.16	0	6,6,6	0.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SO4	1	0
2	B	2	SO4	1	0
2	B	14	SO4	3	0
2	B	12	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	223/227 (98%)	0.26	2 (0%)	84	80	29, 31, 34, 38	0
1	B	221/227 (97%)	0.30	3 (1%)	75	70	29, 31, 34, 38	0
1	C	223/227 (98%)	0.47	9 (4%)	38	28	29, 31, 34, 43	0
All	All	667/681 (97%)	0.34	14 (2%)	63	54	29, 31, 34, 43	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	GLU	2.9
1	C	181	ASP	2.9
1	C	182	SER	2.8
1	C	180	PRO	2.7
1	B	182	SER	2.6
1	C	72	GLY	2.5
1	C	236	LYS	2.5
1	C	75	ARG	2.5
1	B	83	LYS	2.4
1	B	82	SER	2.4
1	C	49	ARG	2.3
1	C	123	CYS	2.1
1	A	182	SER	2.1
1	A	181	ASP	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	239	5/5	0.85	0.40	79,80,80,80	0
2	SO4	B	14	5/5	0.88	0.28	69,69,70,71	0
2	SO4	A	8	5/5	0.91	0.22	65,66,66,67	0
2	SO4	B	12	5/5	0.91	0.46	58,58,59,60	0
2	SO4	A	13	5/5	0.93	0.17	69,69,70,70	0
2	SO4	A	9	5/5	0.93	0.17	50,51,51,52	0
2	SO4	A	7	5/5	0.94	0.30	47,49,50,50	0
2	SO4	B	15	5/5	0.95	0.34	62,63,63,63	0
2	SO4	B	10	5/5	0.96	0.16	56,57,58,58	0
2	SO4	C	4	5/5	0.96	0.18	39,39,41,42	0
2	SO4	C	6	5/5	0.96	0.14	57,58,59,59	0
2	SO4	B	11	5/5	0.96	0.23	59,59,60,62	0
2	SO4	A	5	5/5	0.97	0.12	52,53,54,54	0
2	SO4	B	2	5/5	0.97	0.15	38,38,39,39	0
2	SO4	C	3	5/5	0.98	0.10	32,35,35,38	0
2	SO4	A	1	5/5	0.98	0.10	22,25,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.