



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:58 PM EDT

PDB ID : 3UY8 / pdb_00003uy8
Title : Designed protein KE59 R5_11/5F
Authors : Khersonsky, O.; Kiss, G.; Roethlisberger, D.; Dym, O.; Albeck, S.; Houk, K.N.; Baker, D.; Tawfik, D.S.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2011-12-06
Resolution : 2.41 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

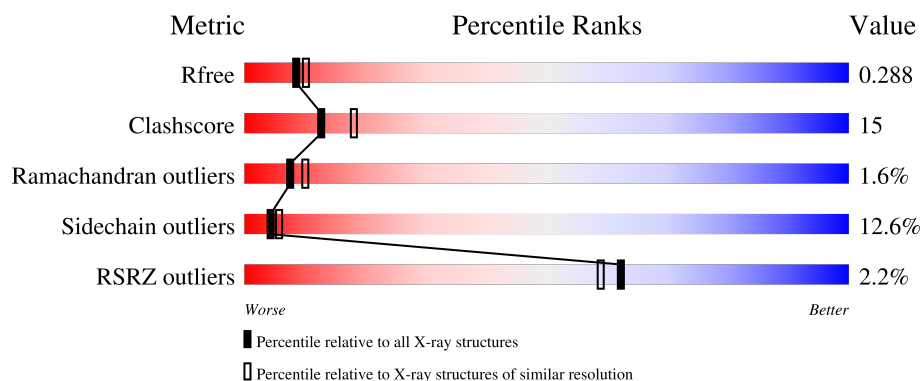
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	247	3% 47% 36% 14% .
1	B	247	2% 58% 29% 11% .

2 Entry composition [i](#)

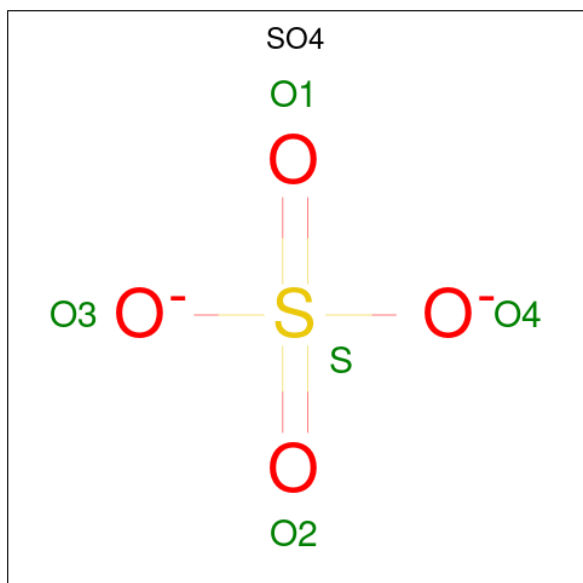
There are 3 unique types of molecules in this entry. The entry contains 3947 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kemp eliminase KE59 R5_11/5F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1970	1261	335	369	5			
1	B	247	Total	C	N	O	S	0	0	0
			1962	1251	335	371	5			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

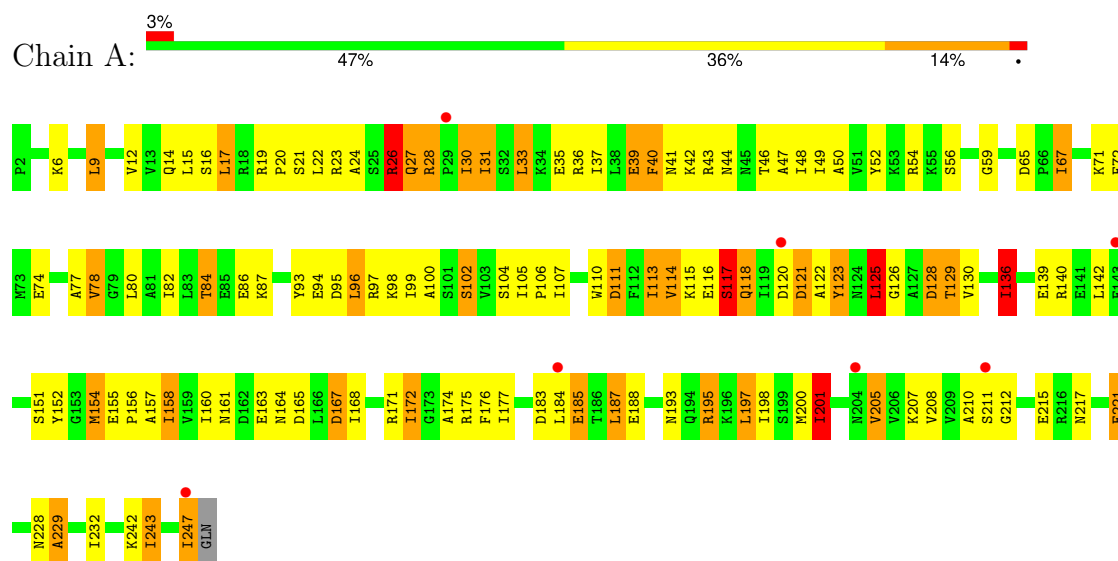
- Molecule 3 is water.

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

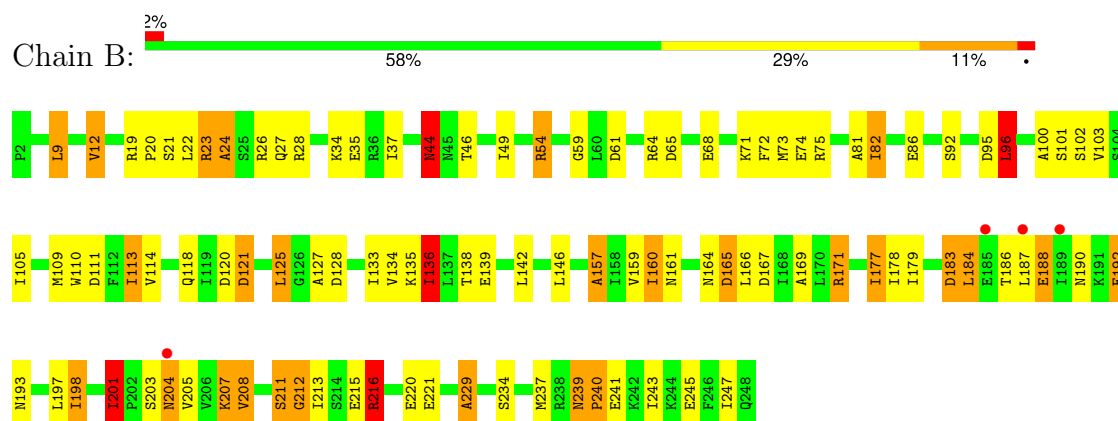
3 Residue-property plots

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: Kemp eliminase KE59 R5_11/5F



• Molecule 1: Kemp eliminase KE59 R5_11/5F



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.96Å 102.73Å 66.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.98 – 2.41 43.98 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.98-2.41) 98.3 (43.98-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.215 , 0.299 0.217 , 0.288	Depositor DCC
R_{free} test set	1201 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 18.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3947	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	2.16	60/2000 (3.0%)	1.70	42/2696 (1.6%)
1	B	2.02	41/1992 (2.1%)	1.68	39/2690 (1.4%)
All	All	2.09	101/3992 (2.5%)	1.69	81/5386 (1.5%)

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

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	GLU	C-O	11.80	1.38	1.24
1	B	211	SER	C-O	10.79	1.36	1.23
1	B	201	ILE	CA-CB	10.61	1.63	1.54
1	A	37	ILE	CA-CB	10.38	1.66	1.54
1	A	107	ILE	CA-CB	9.17	1.65	1.54
1	B	111	ASP	C-O	-8.45	1.16	1.24
1	A	107	ILE	N-CA	-8.36	1.36	1.46
1	A	84	THR	CA-C	-8.34	1.43	1.52
1	A	77	ALA	N-CA	-8.33	1.35	1.45
1	A	117	SER	C-O	8.29	1.34	1.24
1	B	177	ILE	CG1-CD1	7.97	1.82	1.51
1	A	129	THR	CA-CB	7.92	1.66	1.53
1	B	133	ILE	C-O	7.91	1.32	1.24
1	A	125	LEU	CA-C	-7.80	1.42	1.52
1	B	49	ILE	CA-CB	-7.48	1.45	1.53
1	B	103	VAL	CA-C	-7.36	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	ARG	CD-NE	-7.21	1.36	1.46
1	B	128	ASP	C-O	-7.20	1.14	1.24
1	A	151	SER	N-CA	7.17	1.55	1.46
1	A	93	TYR	C-O	7.17	1.32	1.24
1	B	120	ASP	N-CA	7.17	1.54	1.46
1	A	123	TYR	CA-CB	7.15	1.64	1.53
1	A	49	ILE	CA-CB	-7.05	1.45	1.53
1	A	210	ALA	N-CA	6.95	1.54	1.46
1	A	129	THR	C-O	-6.77	1.16	1.23
1	A	47	ALA	C-O	6.70	1.31	1.24
1	B	113	ILE	CA-CB	-6.66	1.46	1.53
1	A	157	ALA	CA-CB	-6.66	1.42	1.53
1	A	121	ASP	CA-C	-6.64	1.44	1.52
1	A	232	ILE	CA-CB	-6.58	1.45	1.54
1	B	105	ILE	C-O	-6.57	1.19	1.24
1	A	120	ASP	N-CA	6.49	1.54	1.46
1	A	243	ILE	CA-C	6.47	1.60	1.52
1	B	229	ALA	CA-CB	6.44	1.64	1.53
1	A	120	ASP	C-O	6.42	1.31	1.24
1	B	96	LEU	C-O	6.37	1.31	1.24
1	B	61	ASP	C-O	6.34	1.31	1.23
1	A	100	ALA	CA-CB	-6.32	1.43	1.53
1	B	102	SER	CA-C	-6.29	1.44	1.52
1	A	71	LYS	CA-C	-6.28	1.44	1.52
1	B	237	MET	CA-C	6.21	1.61	1.52
1	B	86	GLU	CA-C	6.17	1.60	1.52
1	A	106	PRO	C-O	6.16	1.30	1.23
1	B	34	LYS	N-CA	-6.14	1.39	1.46
1	A	9	LEU	C-O	-6.09	1.17	1.24
1	A	118	GLN	CA-C	-6.05	1.44	1.52
1	A	35	GLU	CA-C	-6.03	1.44	1.52
1	A	104	SER	CA-C	5.99	1.61	1.52
1	A	164	ASN	N-CA	5.99	1.53	1.46
1	B	12	VAL	N-CA	-5.99	1.39	1.46
1	A	154	MET	N-CA	5.96	1.52	1.45
1	B	234	SER	CA-C	-5.96	1.44	1.52
1	A	114	VAL	N-CA	5.95	1.53	1.46
1	B	121	ASP	C-O	5.92	1.30	1.24
1	A	111	ASP	C-O	-5.92	1.18	1.24
1	B	100	ALA	N-CA	5.87	1.53	1.46
1	A	221	GLU	CG-CD	5.82	1.66	1.52
1	B	208	VAL	CA-CB	-5.81	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	VAL	CA-C	5.79	1.60	1.52
1	A	39	GLU	N-CA	5.77	1.53	1.46
1	A	205	VAL	C-O	-5.76	1.18	1.24
1	A	86	GLU	C-O	-5.70	1.16	1.23
1	A	198	ILE	N-CA	-5.68	1.39	1.46
1	B	133	ILE	CA-CB	-5.67	1.47	1.53
1	A	136	ILE	CA-CB	5.66	1.61	1.54
1	A	114	VAL	CA-CB	-5.60	1.46	1.54
1	B	101	SER	CA-C	-5.59	1.45	1.52
1	A	16	SER	CA-C	5.54	1.60	1.52
1	B	61	ASP	N-CA	5.54	1.53	1.46
1	A	158	ILE	N-CA	5.50	1.53	1.46
1	A	72	PHE	CA-C	5.49	1.59	1.52
1	A	36	ARG	N-CA	5.46	1.53	1.46
1	A	100	ALA	CA-C	5.45	1.59	1.52
1	A	17	LEU	C-O	5.42	1.30	1.24
1	A	87	LYS	N-CA	-5.42	1.39	1.46
1	A	122	ALA	C-O	5.40	1.30	1.24
1	B	229	ALA	C-O	5.37	1.30	1.23
1	B	109	MET	CA-CB	-5.36	1.45	1.53
1	A	172	ILE	N-CA	5.34	1.52	1.46
1	B	198	ILE	CA-CB	-5.32	1.47	1.54
1	B	146	LEU	C-O	-5.31	1.17	1.24
1	B	234	SER	C-O	-5.31	1.17	1.24
1	A	65	ASP	CA-C	5.29	1.58	1.52
1	B	157	ALA	CA-C	-5.24	1.46	1.52
1	A	229	ALA	C-O	5.23	1.29	1.23
1	B	37	ILE	N-CA	5.16	1.52	1.46
1	A	129	THR	CB-CG2	-5.16	1.35	1.52
1	A	46	THR	C-O	-5.13	1.17	1.23
1	B	159	VAL	CA-CB	-5.12	1.48	1.54
1	A	37	ILE	C-O	5.12	1.29	1.24
1	A	174	ALA	CA-CB	-5.11	1.44	1.53
1	A	52	TYR	C-O	-5.11	1.17	1.24
1	B	102	SER	C-O	-5.11	1.17	1.24
1	A	126	GLY	N-CA	5.10	1.52	1.45
1	B	164	ASN	C-O	5.10	1.30	1.24
1	B	71	LYS	N-CA	5.09	1.52	1.46
1	A	67	ILE	C-O	-5.08	1.18	1.24
1	B	64	ARG	CZ-NH1	5.08	1.39	1.32
1	B	26	ARG	C-O	-5.07	1.17	1.24
1	A	193	ASN	CA-C	5.05	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	THR	C-O	-5.03	1.17	1.23

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASP	N-CA-C	9.30	124.17	113.01
1	B	28	ARG	NE-CZ-NH2	9.21	127.49	119.20
1	A	84	THR	N-CA-C	-8.99	98.67	113.50
1	A	24	ALA	N-CA-C	8.90	122.22	108.96
1	A	87	LYS	N-CA-C	8.66	120.50	111.14
1	A	116	GLU	N-CA-C	8.50	120.55	111.28
1	A	71	LYS	N-CA-C	-8.38	102.10	111.82
1	A	155	GLU	CA-C-N	8.21	127.97	119.76
1	A	155	GLU	C-N-CA	8.21	127.97	119.76
1	B	138	THR	N-CA-C	-7.89	99.90	110.55
1	B	201	ILE	CB-CA-C	7.74	119.11	110.52
1	B	187	LEU	CA-C-N	7.73	135.61	121.70
1	B	187	LEU	C-N-CA	7.73	135.61	121.70
1	B	59	GLY	N-CA-C	7.61	125.99	115.27
1	A	187	LEU	N-CA-C	7.50	120.39	111.02
1	A	28	ARG	N-CA-CB	7.46	117.92	109.49
1	A	123	TYR	N-CA-C	-7.39	103.17	111.07
1	A	201	ILE	CB-CG1-CD1	-7.30	98.47	113.80
1	B	44	ASN	N-CA-C	7.18	126.10	110.80
1	B	101	SER	CA-C-N	-7.01	111.22	122.23
1	B	101	SER	C-N-CA	-7.01	111.22	122.23
1	B	204	ASN	N-CA-C	6.87	125.42	110.80
1	B	198	ILE	N-CA-C	6.78	119.53	111.05
1	A	200	MET	CA-C-N	-6.75	109.64	122.13
1	A	200	MET	C-N-CA	-6.75	109.64	122.13
1	A	221	GLU	N-CA-C	-6.72	103.76	112.23
1	B	188	GLU	N-CA-C	6.58	129.41	111.00
1	A	40	PHE	N-CA-C	-6.52	104.25	111.36
1	B	216	ARG	N-CA-C	6.52	119.39	111.82
1	B	136	ILE	CA-CB-CG2	6.47	121.50	110.50
1	B	198	ILE	CB-CA-C	-6.27	102.44	112.16
1	B	105	ILE	CB-CA-C	6.20	116.58	109.89
1	B	192	GLU	CA-C-N	6.13	130.40	120.60
1	B	192	GLU	C-N-CA	6.13	130.40	120.60
1	A	136	ILE	CA-CB-CG2	6.06	120.80	110.50
1	B	171	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	A	49	ILE	CB-CA-C	-6.04	103.58	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	GLU	N-CA-C	5.95	118.72	111.82
1	A	72	PHE	N-CA-C	5.92	117.82	111.36
1	A	15	LEU	N-CA-C	-5.85	105.04	111.82
1	B	240	PRO	CA-C-N	5.78	128.82	120.38
1	B	240	PRO	C-N-CA	5.78	128.82	120.38
1	A	167	ASP	N-CA-C	-5.76	105.00	111.28
1	A	59	GLY	N-CA-C	5.75	122.61	114.85
1	B	35	GLU	N-CA-C	5.75	117.54	111.28
1	B	134	VAL	CB-CA-C	-5.74	104.53	112.04
1	A	136	ILE	N-CA-C	-5.71	107.94	113.53
1	B	167	ASP	N-CA-C	5.59	117.06	111.07
1	B	121	ASP	CA-C-N	-5.59	112.79	120.28
1	B	121	ASP	C-N-CA	-5.59	112.79	120.28
1	A	26	ARG	N-CA-C	-5.56	102.06	110.28
1	B	171	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	A	33	LEU	N-CA-C	-5.48	105.38	111.36
1	A	152	TYR	N-CA-C	5.48	119.06	112.38
1	B	44	ASN	CA-C-N	5.45	131.51	121.70
1	B	44	ASN	C-N-CA	5.45	131.51	121.70
1	B	74	GLU	N-CA-C	5.41	118.67	111.75
1	B	245	GLU	N-CA-C	-5.41	105.39	111.28
1	A	93	TYR	N-CA-C	5.37	118.62	111.75
1	A	22	LEU	N-CA-C	5.33	118.74	110.17
1	A	121	ASP	CA-C-N	-5.32	113.16	120.28
1	A	121	ASP	C-N-CA	-5.32	113.16	120.28
1	A	151	SER	N-CA-CB	5.29	118.00	110.06
1	A	157	ALA	CA-C-N	-5.29	116.26	122.93
1	A	157	ALA	C-N-CA	-5.29	116.26	122.93
1	B	165	ASP	N-CA-C	-5.29	105.59	111.36
1	A	193	ASN	CB-CA-C	5.20	118.77	110.09
1	B	111	ASP	N-CA-C	-5.19	101.39	108.24
1	B	201	ILE	CA-CB-CG2	5.18	119.30	110.50
1	A	197	LEU	N-CA-C	5.14	117.28	111.11
1	A	100	ALA	N-CA-C	5.14	116.88	111.28
1	A	176	PHE	CB-CA-C	5.13	118.11	110.62
1	B	179	ILE	N-CA-CB	5.09	116.80	111.00
1	B	92	SER	CA-C-N	5.09	127.10	120.28
1	B	92	SER	C-N-CA	5.09	127.10	120.28
1	A	31	ILE	CB-CA-C	-5.07	103.83	110.98
1	A	28	ARG	CA-C-N	-5.04	114.79	120.14
1	A	28	ARG	C-N-CA	-5.04	114.79	120.14
1	A	97	ARG	N-CA-C	5.04	117.16	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	VAL	CB-CA-C	-5.04	101.79	110.30
1	B	169	ALA	N-CA-C	5.03	116.76	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	203	SER	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	1970	0	2027	68	0
1	B	1962	0	1991	55	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
All	All	3947	0	4018	121	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 15.

All (121) 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:B:177:ILE:CD1	1:B:177:ILE:CG1	1.82	1.57
1:A:21:SER:HB2	1:A:121:ASP:OD1	1.39	1.18
1:A:26:ARG:CA	1:A:27:GLN:HB2	1.70	1.18
1:A:26:ARG:HA	1:A:27:GLN:CB	1.77	1.14
1:A:195:ARG:HH21	1:A:195:ARG:HG3	1.21	1.00
1:B:23:ARG:HG2	1:B:23:ARG:O	1.64	0.98
1:B:23:ARG:HA	1:B:24:ALA:HB3	1.46	0.93
1:B:81:ALA:C	1:B:82:ILE:HD13	1.94	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:SER:CB	1:A:121:ASP:OD1	2.18	0.91
1:A:201:ILE:HD11	1:A:207:LYS:HD3	1.53	0.87
1:A:26:ARG:HA	1:A:27:GLN:HB2	0.90	0.85
1:A:95:ASP:O	1:A:99:ILE:HG13	1.79	0.82
1:A:9:LEU:HD12	1:A:185:GLU:HG3	1.64	0.80
1:A:201:ILE:HD11	1:A:207:LYS:CD	2.10	0.79
1:A:187:LEU:N	1:A:188:GLU:HB2	1.98	0.79
1:A:201:ILE:CD1	1:A:207:LYS:HD3	2.12	0.79
1:A:44:ASN:HD21	1:B:27:GLN:H	1.30	0.78
1:B:23:ARG:CA	1:B:24:ALA:HB3	2.13	0.78
1:A:44:ASN:ND2	1:B:27:GLN:H	1.84	0.76
1:B:198:ILE:HG22	1:B:198:ILE:O	1.86	0.75
1:B:9:LEU:HD21	1:B:136:ILE:HD11	1.67	0.74
1:A:195:ARG:HH21	1:A:195:ARG:CG	2.00	0.72
1:B:198:ILE:O	1:B:198:ILE:CG2	2.36	0.72
1:B:208:VAL:HG22	1:B:229:ALA:HB3	1.71	0.72
1:B:22:LEU:CD1	1:B:125:LEU:HD11	2.22	0.68
1:B:23:ARG:CA	1:B:24:ALA:CB	2.71	0.68
1:A:54:ARG:NH2	1:A:95:ASP:OD2	2.26	0.67
1:A:195:ARG:HG3	1:A:195:ARG:NH2	2.02	0.67
1:B:201:ILE:HD11	1:B:205:VAL:HB	1.76	0.66
1:B:114:VAL:H	1:B:118:GLN:NE2	1.93	0.66
1:A:115:LYS:HG2	1:A:118:GLN:HE21	1.61	0.65
1:A:114:VAL:H	1:A:118:GLN:NE2	1.95	0.64
1:A:96:LEU:HD13	1:A:125:LEU:HB3	1.80	0.64
1:A:139:GLU:HG3	1:A:168:ILE:HG23	1.80	0.64
1:A:115:LYS:HE3	1:A:117:SER:OG	1.97	0.63
1:A:19:ARG:HD2	1:A:20:PRO:HD2	1.81	0.62
1:B:114:VAL:HG22	1:B:118:GLN:HE22	1.65	0.61
1:A:82:ILE:HD12	1:A:99:ILE:HD12	1.83	0.61
1:B:139:GLU:OE1	1:B:171:ARG:NH1	2.32	0.61
1:A:114:VAL:HG22	1:A:118:GLN:HE22	1.65	0.60
1:A:177:ILE:HD12	1:A:205:VAL:HG11	1.84	0.60
1:B:81:ALA:O	1:B:82:ILE:HD13	2.01	0.60
1:B:22:LEU:HD13	1:B:125:LEU:HD11	1.83	0.59
1:B:23:ARG:O	1:B:23:ARG:CG	2.42	0.57
1:A:39:GLU:O	1:A:43:ARG:HG3	2.04	0.56
1:A:67:ILE:HD11	1:A:98:LYS:HB3	1.88	0.56
1:A:26:ARG:HD3	1:A:123:TYR:CZ	2.40	0.56
1:A:98:LYS:O	1:A:102:SER:OG	2.23	0.55
1:B:201:ILE:HD12	1:B:207:LYS:CG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASN:O	1:B:240:PRO:C	2.47	0.55
1:B:9:LEU:CD2	1:B:136:ILE:HD11	2.38	0.54
1:B:211:SER:C	1:B:213:ILE:H	2.15	0.54
1:A:114:VAL:CG2	1:A:118:GLN:HE22	2.21	0.54
1:B:190:ASN:HD21	1:B:192:GLU:HG2	1.73	0.54
1:B:21:SER:OG	1:B:121:ASP:OD1	2.19	0.54
1:B:135:LYS:NZ	1:B:165:ASP:OD1	2.41	0.53
1:A:201:ILE:HD11	1:A:207:LYS:CG	2.37	0.53
1:B:160:ILE:HB	1:B:165:ASP:HB2	1.90	0.53
1:A:201:ILE:O	1:A:201:ILE:HD13	2.09	0.53
1:A:217:ASN:O	1:A:221:GLU:HG3	2.10	0.52
1:A:40:PHE:CD2	1:A:78:VAL:HG23	2.43	0.52
1:B:211:SER:OG	1:B:212:GLY:N	2.41	0.52
1:A:201:ILE:HD13	1:A:201:ILE:C	2.35	0.52
1:B:183:ASP:OD1	1:B:186:THR:HG23	2.08	0.52
1:A:30:ILE:HD11	1:A:123:TYR:CE1	2.46	0.51
1:A:21:SER:HB3	1:A:121:ASP:OD2	2.10	0.51
1:A:21:SER:CB	1:A:121:ASP:CG	2.83	0.51
1:A:9:LEU:HD22	1:A:136:ILE:HD11	1.93	0.51
1:A:154:MET:O	1:A:156:PRO:HD3	2.11	0.50
1:B:114:VAL:H	1:B:118:GLN:HE22	1.58	0.50
1:B:44:ASN:O	1:B:44:ASN:OD1	2.30	0.50
1:A:247:ILE:CD1	1:A:247:ILE:N	2.75	0.49
1:A:96:LEU:HD13	1:A:125:LEU:CB	2.42	0.49
1:B:65:ASP:HB3	1:B:68:GLU:HG3	1.95	0.49
1:B:201:ILE:HD12	1:B:207:LYS:HG2	1.95	0.48
1:A:41:ASN:ND2	1:A:228:ASN:HD22	2.11	0.48
1:A:195:ARG:CG	1:A:195:ARG:NH2	2.67	0.47
1:A:50:ALA:O	1:A:80:LEU:HA	2.14	0.47
1:A:201:ILE:HD11	1:A:207:LYS:NZ	2.29	0.46
1:A:211:SER:O	1:A:212:GLY:C	2.58	0.46
1:B:9:LEU:HD23	1:B:9:LEU:O	2.15	0.46
1:A:31:ILE:O	1:A:128:ASP:HB3	2.15	0.45
1:A:115:LYS:HG2	1:A:118:GLN:NE2	2.29	0.45
1:A:242:LYS:O	1:A:243:ILE:C	2.59	0.45
1:B:201:ILE:HD11	1:B:205:VAL:CB	2.46	0.45
1:B:201:ILE:C	1:B:201:ILE:HD13	2.41	0.45
1:B:82:ILE:HD13	1:B:82:ILE:N	2.28	0.45
1:B:22:LEU:HD12	1:B:125:LEU:HD11	1.96	0.45
1:B:177:ILE:CD1	1:B:177:ILE:CB	2.81	0.45
1:B:72:PHE:C	1:B:72:PHE:CD2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:OG1	1:A:111:ASP:OD2	2.26	0.45
1:B:19:ARG:HA	1:B:20:PRO:HD3	1.73	0.45
1:B:157:ALA:HB1	1:B:178:ILE:HG13	1.99	0.45
1:A:208:VAL:HG22	1:A:229:ALA:HB3	1.98	0.44
1:A:247:ILE:N	1:A:247:ILE:HD13	2.33	0.44
1:A:160:ILE:HB	1:A:165:ASP:HB3	1.99	0.44
1:A:167:ASP:OD2	1:A:171:ARG:NH2	2.51	0.43
1:B:211:SER:C	1:B:213:ILE:N	2.76	0.43
1:B:96:LEU:HD11	1:B:127:ALA:HB2	2.01	0.43
1:B:216:ARG:O	1:B:216:ARG:HG3	2.17	0.43
1:B:114:VAL:CG2	1:B:118:GLN:HE22	2.29	0.43
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.85	0.43
1:B:201:ILE:HD11	1:B:205:VAL:CG1	2.48	0.43
1:A:113:ILE:HD12	1:A:130:VAL:HB	2.00	0.43
1:A:187:LEU:CA	1:A:188:GLU:HB2	2.50	0.42
1:B:9:LEU:HD11	1:B:184:LEU:HB3	2.02	0.42
1:B:23:ARG:N	1:B:24:ALA:CB	2.82	0.42
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.63	0.42
1:A:41:ASN:HD21	1:A:228:ASN:HD22	1.67	0.42
1:A:54:ARG:HH22	1:A:95:ASP:CG	2.26	0.42
1:A:183:ASP:HB3	1:A:187:LEU:H	1.85	0.42
1:B:54:ARG:NH2	1:B:95:ASP:OD2	2.40	0.42
1:A:17:LEU:HA	1:A:17:LEU:HD23	1.85	0.41
1:A:94:GLU:O	1:A:98:LYS:HG3	2.21	0.41
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.91	0.41
1:B:216:ARG:NH2	1:B:220:GLU:OE1	2.54	0.41
1:A:201:ILE:HG23	1:A:201:ILE:HD12	1.73	0.41
1:B:73:MET:SD	1:B:243:ILE:HD12	2.61	0.40
1:A:139:GLU:HG3	1:A:168:ILE:CG2	2.50	0.40
1:B:166:LEU:O	1:B:166:LEU:HD12	2.20	0.40
1:A:80:LEU:HD12	1:A:105:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/247 (99%)	227 (93%)	14 (6%)	3 (1%)	10	15
1	B	245/247 (99%)	230 (94%)	10 (4%)	5 (2%)	6	7
All	All	489/494 (99%)	457 (94%)	24 (5%)	8 (2%)	7	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	B	24	ALA
1	B	204	ASN
1	A	74	GLU
1	B	44	ASN
1	B	188	GLU
1	B	212	GLY
1	A	30	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	215/221 (97%)	185 (86%)	30 (14%)	3	4
1	B	213/221 (96%)	189 (89%)	24 (11%)	5	8
All	All	428/442 (97%)	374 (87%)	54 (13%)	4	6

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

Mol	Chain	Res	Type
1	A	6	LYS
1	A	14	GLN
1	A	23	ARG
1	A	26	ARG
1	A	28	ARG

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Mol	Chain	Res	Type
1	A	33	LEU
1	A	42	LYS
1	A	48	ILE
1	A	56	SER
1	A	78	VAL
1	A	96	LEU
1	A	102	SER
1	A	110	TRP
1	A	113	ILE
1	A	117	SER
1	A	125	LEU
1	A	129	THR
1	A	136	ILE
1	A	140	ARG
1	A	142	LEU
1	A	158	ILE
1	A	161	ASN
1	A	163	GLU
1	A	172	ILE
1	A	175	ARG
1	A	184	LEU
1	A	195	ARG
1	A	201	ILE
1	A	215	GLU
1	A	247	ILE
1	B	9	LEU
1	B	12	VAL
1	B	23	ARG
1	B	75	ARG
1	B	82	ILE
1	B	96	LEU
1	B	110	TRP
1	B	113	ILE
1	B	125	LEU
1	B	136	ILE
1	B	142	LEU
1	B	160	ILE
1	B	161	ASN
1	B	183	ASP
1	B	184	LEU
1	B	193	ASN
1	B	201	ILE

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Mol	Chain	Res	Type
1	B	207	LYS
1	B	215	GLU
1	B	216	ARG
1	B	221	GLU
1	B	239	ASN
1	B	241	GLU
1	B	247	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	44	ASN
1	A	118	GLN
1	A	124	ASN
1	A	161	ASN
1	B	44	ASN
1	B	118	GLN
1	B	124	ASN
1	B	161	ASN
1	B	190	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	B	1	-	4,4,4	0.48	0	6,6,6	0.50	0
2	SO4	A	249	-	4,4,4	0.26	0	6,6,6	0.61	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	246/247 (99%)	0.09	7 (2%) 55 51	22, 42, 66, 88	0
1	B	247/247 (100%)	-0.07	4 (1%) 70 67	24, 41, 68, 87	0
All	All	493/494 (99%)	0.01	11 (2%) 62 59	22, 41, 68, 88	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	ILE	3.6
1	B	187	LEU	3.1
1	A	204	ASN	2.8
1	A	184	LEU	2.4
1	A	143	GLU	2.4
1	B	204	ASN	2.3
1	B	189	ILE	2.2
1	A	29	PRO	2.1
1	B	185	GLU	2.0
1	A	120	ASP	2.0
1	A	211	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	249	5/5	0.66	0.17	126,127,128,128	0
2	SO4	B	1	5/5	0.71	0.14	88,90,92,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.