



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:15 AM EDT

PDB ID : 4U2Q / pdb_00004u2q
Title : Full-length AMPA subtype ionotropic glutamate receptor GluA2 in complex with partial agonist kainate
Authors : Duerr, K.L.; Chen, L.; Gouaux, E.
Deposited on : 2014-07-17
Resolution : 3.52 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

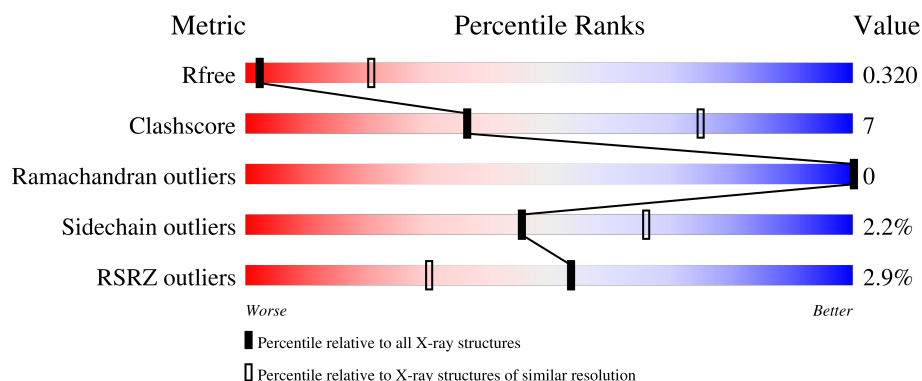
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	824	0% 72% 14% • 12%
1	B	824	2% 75% 15% • 9%
1	C	824	3% 75% 15% • 10%
1	D	824	4% 73% 17% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22448 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5410	3480	890	1017	23			
1	B	746	Total	C	N	O	S	0	0	0
			5674	3649	937	1063	25			
1	C	744	Total	C	N	O	S	0	0	0
			5631	3615	933	1057	26			
1	D	749	Total	C	N	O	S	0	0	0
			5631	3616	932	1058	25			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLU	ASN	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	?	-	GLY	deletion	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	528	ALA	CYS	conflict	UNP P19491
A	585	PHE	MET	conflict	UNP P19491
A	589	ALA	CYS	conflict	UNP P19491
A	598	ALA	GLY	conflict	UNP P19491
A	602	ALA	GLY	conflict	UNP P19491
A	815	ALA	CYS	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	239	GLU	ASN	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491

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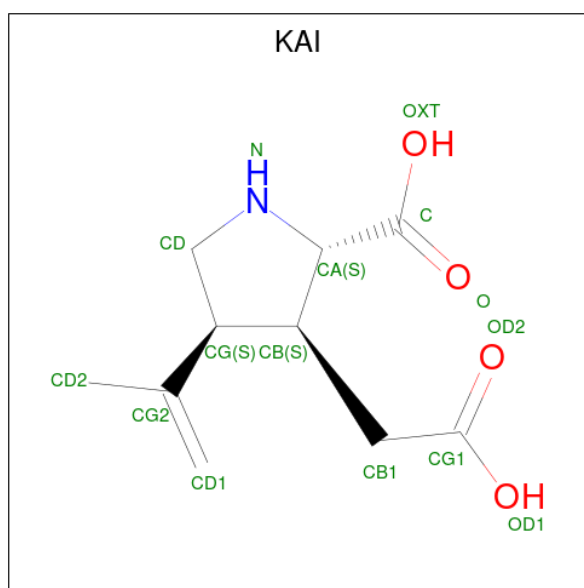
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	528	ALA	CYS	conflict	UNP P19491
B	585	PHE	MET	conflict	UNP P19491
B	589	ALA	CYS	conflict	UNP P19491
B	598	ALA	GLY	conflict	UNP P19491
B	602	ALA	GLY	conflict	UNP P19491
B	815	ALA	CYS	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	239	GLU	ASN	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	?	-	GLY	deletion	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	528	ALA	CYS	conflict	UNP P19491
C	585	PHE	MET	conflict	UNP P19491
C	589	ALA	CYS	conflict	UNP P19491
C	598	ALA	GLY	conflict	UNP P19491
C	602	ALA	GLY	conflict	UNP P19491
C	815	ALA	CYS	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	239	GLU	ASN	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	?	-	GLY	deletion	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	528	ALA	CYS	conflict	UNP P19491
D	585	PHE	MET	conflict	UNP P19491

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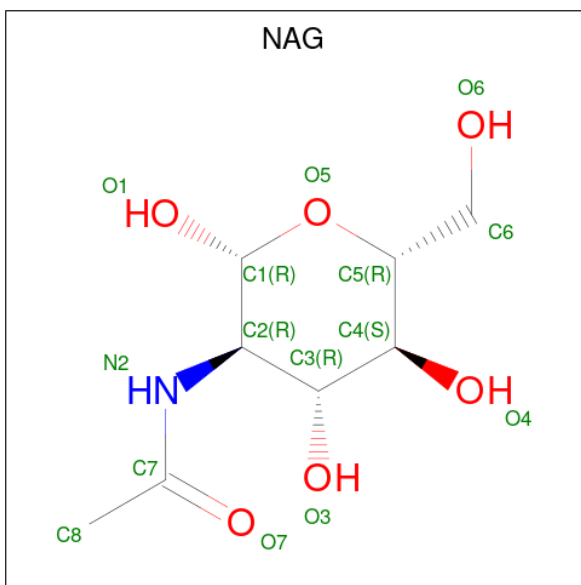
Chain	Residue	Modelled	Actual	Comment	Reference
D	589	ALA	CYS	conflict	UNP P19491
D	598	ALA	GLY	conflict	UNP P19491
D	602	ALA	GLY	conflict	UNP P19491
D	815	ALA	CYS	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is 3-(CARBOXYMETHYL)-4-ISOPROPENYLPROLINE (CCD ID: KAI) (formula: $C_{10}H_{15}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

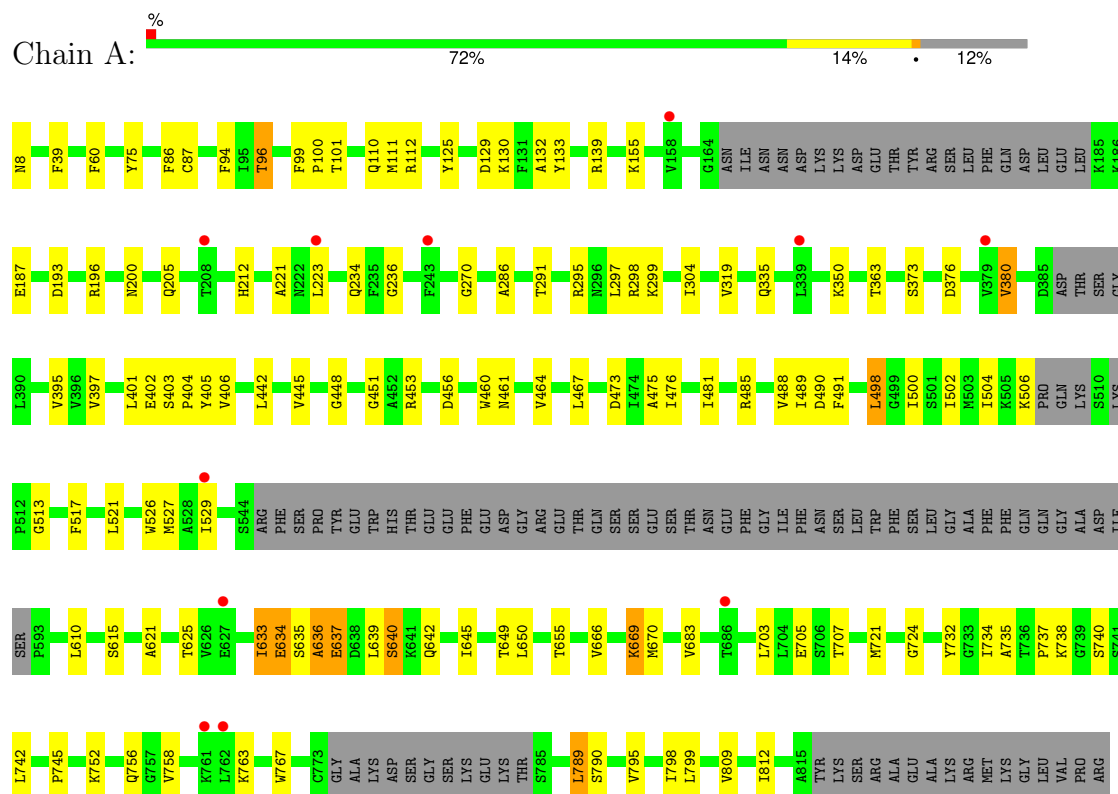


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

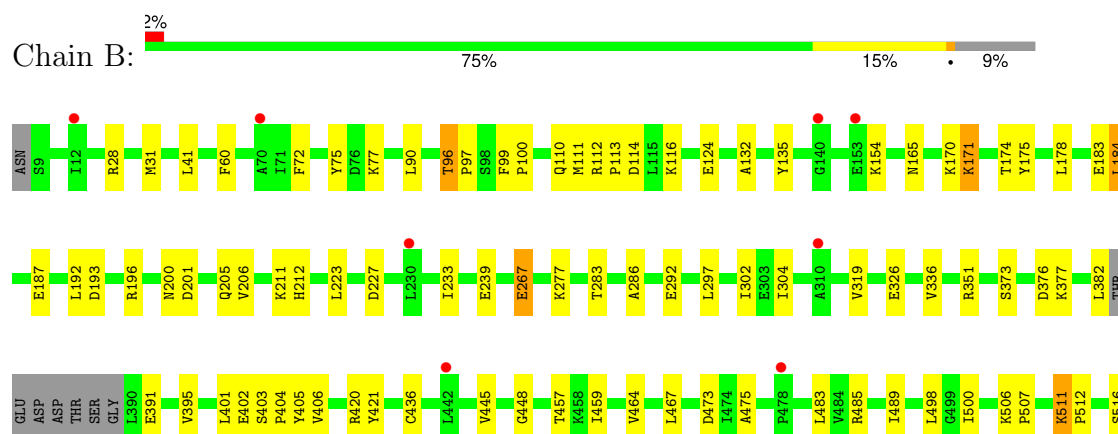
3 Residue-property plots

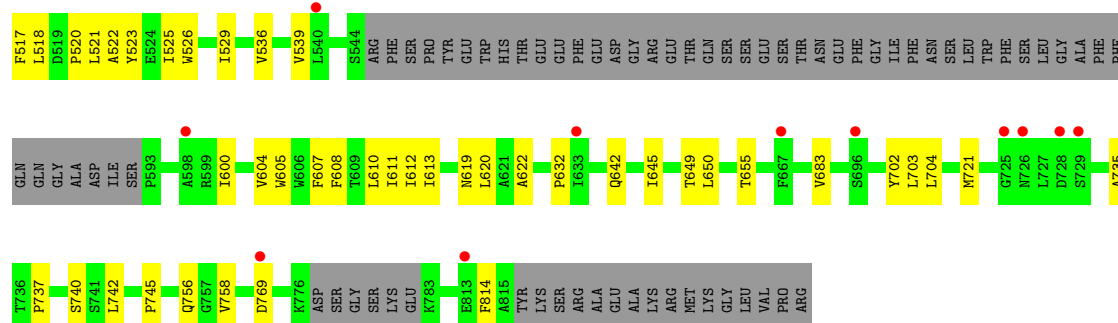
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate receptor 2

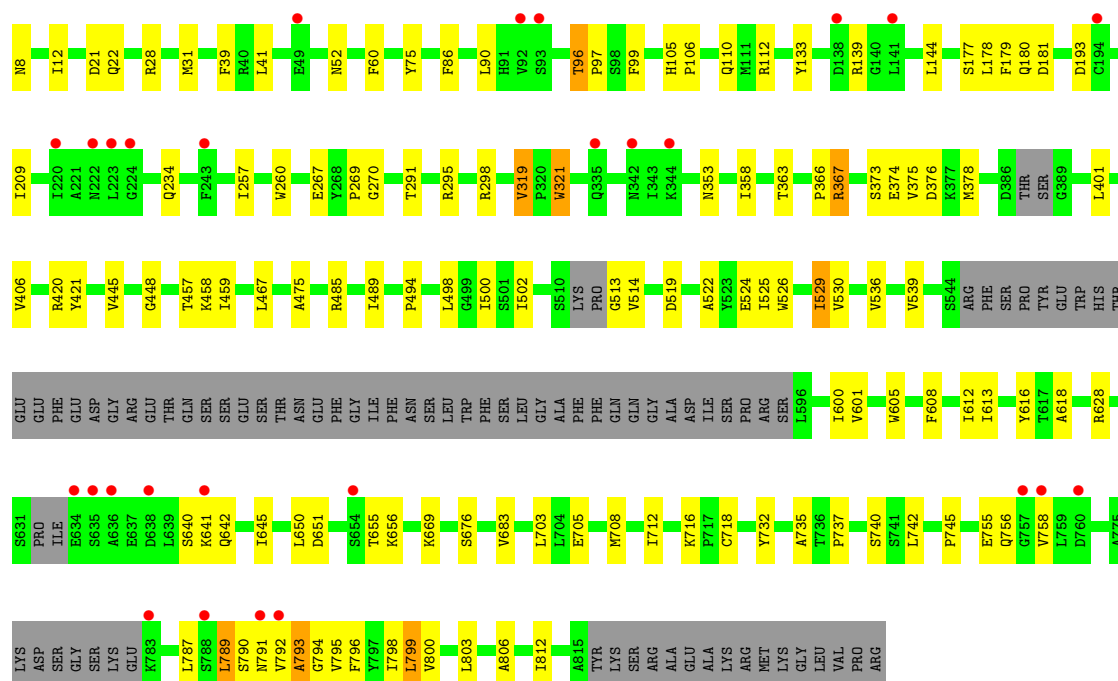
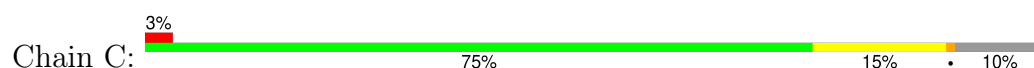


• Molecule 1: Glutamate receptor 2

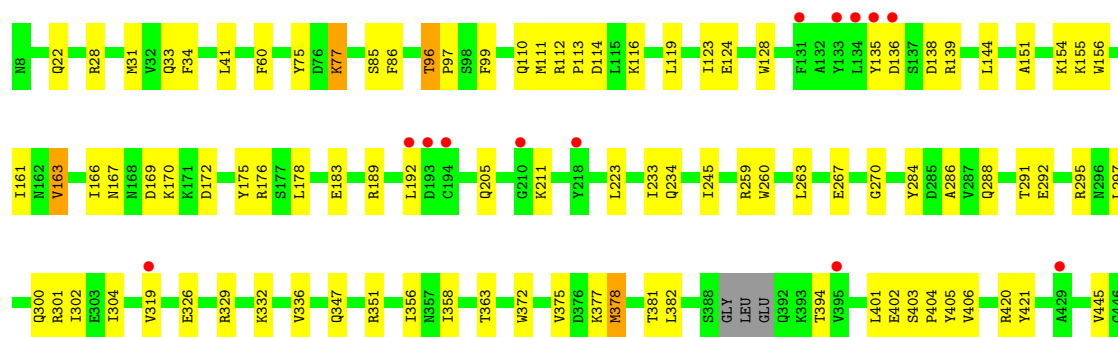


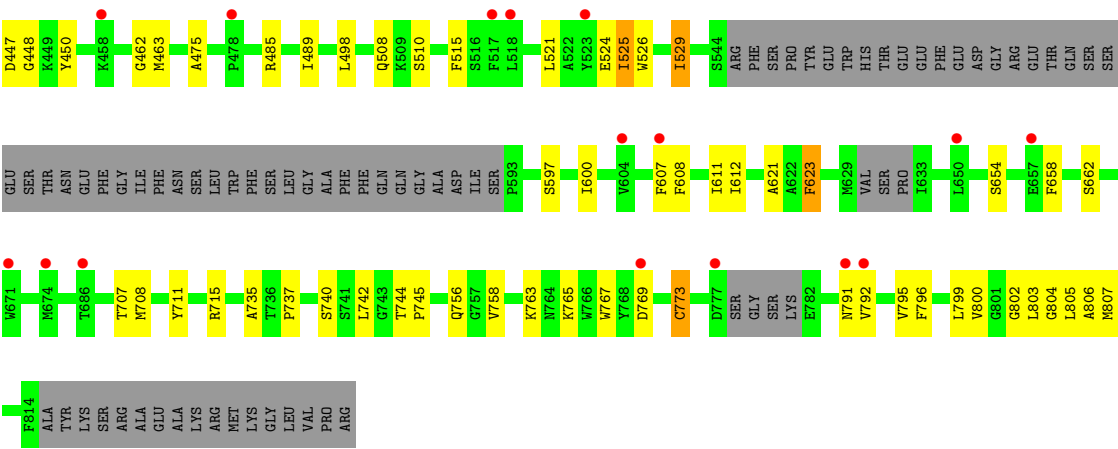


• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.94Å 148.65Å 337.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.08 – 3.52 83.08 – 3.52	Depositor EDS
% Data completeness (in resolution range)	60.6 (83.08-3.52) 60.6 (83.08-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.269 , 0.318 0.270 , 0.320	Depositor DCC
R_{free} test set	2005 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	126.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 203.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22448	wwPDB-VP
Average B, all atoms (Å ²)	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: NAG, KAI

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	0.33	0/5521	0.80	10/7493 (0.1%)
1	B	0.31	0/5792	0.78	4/7847 (0.1%)
1	C	0.32	0/5745	0.79	7/7785 (0.1%)
1	D	0.33	0/5748	0.79	10/7800 (0.1%)
All	All	0.32	0/22806	0.79	31/30925 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	VAL	N-CA-C	7.59	117.66	110.53
1	C	519	ASP	CA-C-N	-7.50	111.98	119.56
1	C	519	ASP	C-N-CA	-7.50	111.98	119.56
1	D	96	THR	CA-C-N	6.89	127.49	120.04
1	D	96	THR	C-N-CA	6.89	127.49	120.04
1	B	96	THR	CA-C-N	6.63	127.20	120.04
1	B	96	THR	C-N-CA	6.63	127.20	120.04
1	D	161	ILE	N-CA-C	6.56	117.57	108.12
1	C	676	SER	N-CA-C	6.52	120.94	112.92
1	D	521	LEU	N-CA-C	6.48	120.08	109.06
1	A	636	ALA	N-CA-C	-6.45	104.90	112.89
1	C	96	THR	CA-C-N	6.27	126.81	120.04
1	C	96	THR	C-N-CA	6.27	126.81	120.04
1	A	96	THR	CA-C-N	6.24	126.78	120.04
1	A	96	THR	C-N-CA	6.24	126.78	120.04
1	B	171	LYS	N-CA-C	6.16	118.08	111.36
1	D	270	GLY	CA-C-N	-5.82	114.99	122.79
1	D	270	GLY	C-N-CA	-5.82	114.99	122.79
1	A	640	SER	N-CA-C	-5.82	105.07	111.82
1	C	319	VAL	N-CA-C	5.82	113.83	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	804	GLY	N-CA-C	-5.68	105.50	112.77
1	A	634	GLU	N-CA-C	-5.66	106.33	113.18
1	A	270	GLY	CA-C-N	-5.64	115.23	122.79
1	A	270	GLY	C-N-CA	-5.64	115.23	122.79
1	C	793	ALA	N-CA-C	5.59	119.28	112.23
1	A	637	GLU	N-CA-C	-5.54	105.26	112.23
1	A	380	VAL	N-CA-C	5.39	115.62	107.75
1	D	524	GLU	N-CA-C	5.35	117.11	111.28
1	D	163	VAL	N-CA-C	5.29	118.07	112.83
1	B	377	LYS	CB-CA-C	-5.04	109.28	116.34
1	D	791	ASN	N-CA-C	5.02	119.00	112.13

There are no chirality outliers.

There are no planarity outliers.

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	5410	0	5189	79	0
1	B	5674	0	5525	86	0
1	C	5631	0	5419	89	0
1	D	5631	0	5392	87	0
2	A	15	0	13	1	0
2	B	15	0	13	2	0
2	C	15	0	13	2	0
2	D	15	0	13	3	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	3	0
All	All	22448	0	21616	317	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 7.

All (317) 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:183:GLU:OE1	1:B:211:LYS:NZ	2.00	0.94
1:B:522:ALA:HB3	1:B:525:ILE:HG13	1.66	0.78
1:B:520:PRO:HA	1:B:619:ASN:HD22	1.48	0.78
1:A:521:LEU:HB3	1:A:526:TRP:HE1	1.48	0.78
1:D:302:ILE:HG21	1:D:326:GLU:HG2	1.69	0.74
1:C:601:VAL:HG22	1:D:803:LEU:HB2	1.70	0.73
1:D:381:THR:HG22	1:D:382:LEU:H	1.54	0.70
1:D:99:PHE:HA	1:D:112:ARG:HD2	1.73	0.70
1:C:28:ARG:NH2	1:C:267:GLU:OE2	2.25	0.69
1:A:196:ARG:O	1:A:200:ASN:ND2	2.26	0.68
1:C:8:ASN:HB3	1:C:298:ARG:HH22	1.57	0.68
1:B:600:ILE:HD11	1:C:806:ALA:HB2	1.76	0.68
1:B:756:GLN:HG3	1:B:758:VAL:HG23	1.77	0.67
1:D:420:ARG:NH1	1:D:421:TYR:OH	2.28	0.66
1:D:756:GLN:HG3	1:D:758:VAL:HG23	1.77	0.66
1:C:640:SER:HB2	1:C:669:LYS:HD2	1.76	0.66
1:C:500:ILE:HD13	1:C:655:THR:HG23	1.76	0.66
1:A:639:LEU:O	1:A:642:GLN:HG3	1.95	0.66
1:B:420:ARG:NH1	1:B:421:TYR:OH	2.29	0.66
1:C:367:ARG:NH1	1:C:367:ARG:HA	2.11	0.65
1:B:619:ASN:OD1	1:C:628:ARG:NH2	2.23	0.65
1:A:475:ALA:HB3	1:A:735:ALA:HB3	1.78	0.65
1:C:641:LYS:O	1:D:773:CYS:HA	1.98	0.64
1:B:622:ALA:HB1	1:C:628:ARG:HG3	1.80	0.63
1:C:642:GLN:NE2	1:C:645:ILE:O	2.31	0.63
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.81	0.63
1:A:132:ALA:HB2	1:A:187:GLU:HG2	1.80	0.62
1:A:506:LYS:HG2	1:A:721:MET:HE3	1.79	0.62
1:B:521:LEU:O	1:B:526:TRP:NE1	2.33	0.62
1:B:196:ARG:HH11	1:B:200:ASN:HD21	1.48	0.61
1:A:756:GLN:HG3	1:A:758:VAL:HG23	1.81	0.61
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.83	0.61
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.83	0.61
1:A:129:ASP:OD1	1:A:130:LYS:N	2.33	0.61
1:A:633:ILE:HG13	1:A:724:GLY:HA3	1.83	0.61
1:C:139:ARG:NH2	1:C:193:ASP:OD1	2.33	0.61
1:C:366:PRO:O	1:C:367:ARG:NH1	2.34	0.61
1:D:737:PRO:HG2	1:D:740:SER:HB2	1.82	0.61
1:B:506:LYS:HG2	1:B:721:MET:HE3	1.83	0.61
1:B:302:ILE:HG21	1:B:326:GLU:HG2	1.83	0.61
1:A:8:ASN:HB3	1:A:298:ARG:HH22	1.66	0.61
1:D:175:TYR:HD2	1:D:205:GLN:HG3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:GLN:O	1:D:301:ARG:HG2	2.01	0.60
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.83	0.60
1:B:742:LEU:C	1:B:745:PRO:HD2	2.27	0.60
1:D:475:ALA:HB3	1:D:735:ALA:HB3	1.83	0.60
1:D:332:LYS:HD3	1:D:347:GLN:HA	1.84	0.60
1:B:112:ARG:HG3	1:B:223:LEU:HD11	1.84	0.59
1:B:99:PHE:HA	1:B:112:ARG:HD2	1.84	0.59
1:C:529:ILE:HG12	1:C:608:PHE:CZ	2.38	0.59
1:D:77:LYS:HG2	1:D:138:ASP:HA	1.84	0.59
1:D:136:ASP:OD2	1:D:139:ARG:NH1	2.35	0.59
1:A:633:ILE:HG23	1:A:634:GLU:H	1.68	0.58
1:B:373:SER:HB3	1:B:376:ASP:HB2	1.85	0.58
1:B:522:ALA:HB2	1:C:787:LEU:HD22	1.84	0.58
1:D:742:LEU:C	1:D:745:PRO:HD2	2.29	0.58
1:C:756:GLN:HG3	1:C:758:VAL:HG23	1.85	0.57
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.85	0.57
1:B:529:ILE:HG13	1:B:608:PHE:HZ	1.70	0.57
1:A:155:LYS:HE3	1:B:184:LEU:HD11	1.87	0.57
1:A:500:ILE:HD13	1:A:655:THR:HG23	1.87	0.57
1:B:132:ALA:HB2	1:B:187:GLU:HG2	1.88	0.56
1:B:175:TYR:HB3	1:B:205:GLN:HG2	1.86	0.56
1:A:737:PRO:HG2	1:A:740:SER:HB2	1.85	0.56
1:B:650:LEU:HD23	1:B:683:VAL:HG23	1.86	0.56
1:D:234:GLN:NE2	1:D:363:THR:O	2.38	0.56
1:A:395:VAL:HG13	1:A:473:ASP:HB2	1.88	0.56
1:C:600:ILE:HD11	1:D:806:ALA:HB2	1.87	0.56
1:D:135:TYR:CE2	1:D:144:LEU:HD22	2.41	0.56
1:A:795:VAL:O	1:A:798:ILE:HG22	2.06	0.55
1:D:802:GLY:O	1:D:805:LEU:HB3	2.05	0.55
1:B:382:LEU:HD23	1:B:382:LEU:H	1.71	0.55
1:B:401:LEU:HD23	1:B:406:VAL:HG12	1.87	0.55
1:C:790:SER:HA	1:C:793:ALA:HB3	1.88	0.55
1:D:658:PHE:O	1:D:662:SER:HB3	2.07	0.55
1:C:737:PRO:HG2	1:C:740:SER:HB2	1.88	0.54
1:A:193:ASP:HA	1:A:221:ALA:HB3	1.89	0.54
1:A:610:LEU:HD11	1:B:613:ILE:HG21	1.88	0.54
1:D:175:TYR:O	1:D:178:LEU:HG	2.07	0.54
1:D:292:GLU:HG3	1:D:336:VAL:HG11	1.89	0.54
1:B:500:ILE:HD13	1:B:655:THR:HG23	1.90	0.54
1:B:165:ASN:O	1:B:165:ASN:ND2	2.40	0.54
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASP:HB3	1:C:269:PRO:HB2	1.91	0.53
1:B:206:VAL:HG12	1:B:212:HIS:HB3	1.91	0.52
1:D:31:MET:HE1	1:D:41:LEU:HB2	1.91	0.52
1:C:358:ILE:HG12	1:C:378:MET:HE1	1.91	0.52
1:C:522:ALA:C	1:C:524:GLU:H	2.17	0.52
1:C:650:LEU:HD23	1:C:683:VAL:HG23	1.91	0.52
1:C:796:PHE:O	1:C:800:VAL:HG23	2.09	0.52
1:A:621:ALA:O	1:A:625:THR:OG1	2.25	0.52
1:D:172:ASP:HB3	1:D:205:GLN:HE21	1.73	0.52
1:D:172:ASP:HB3	1:D:205:GLN:NE2	2.25	0.52
1:D:515:PHE:HB3	1:D:795:VAL:HB	1.92	0.52
1:C:618:ALA:HA	1:D:621:ALA:HB2	1.91	0.52
1:A:445:VAL:HG13	1:A:448:GLY:HA2	1.92	0.52
1:C:373:SER:HB3	1:C:376:ASP:HB2	1.91	0.52
1:D:707:THR:OG1	1:D:708:MET:SD	2.66	0.52
1:B:650:LEU:HD13	2:B:901:KAI:HD23	1.91	0.51
1:C:60:PHE:HE2	1:C:90:LEU:HD12	1.76	0.51
1:C:75:TYR:CE2	1:C:96:THR:HG21	2.45	0.51
1:A:789:LEU:HD21	1:D:525:ILE:HB	1.91	0.51
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.92	0.51
1:D:135:TYR:CZ	1:D:144:LEU:HD22	2.46	0.51
1:C:321:TRP:H	1:C:321:TRP:CD1	2.28	0.51
1:C:133:TYR:OH	1:C:193:ASP:OD2	2.26	0.51
1:B:525:ILE:HD11	1:C:789:LEU:HA	1.94	0.50
1:C:467:LEU:HG	1:C:737:PRO:HD3	1.93	0.50
1:A:669:LYS:NZ	1:B:769:ASP:O	2.34	0.50
1:C:526:TRP:O	1:C:530:VAL:HB	2.12	0.50
1:B:539:VAL:HG21	1:C:803:LEU:HD13	1.93	0.50
1:B:610:LEU:HD11	1:C:613:ILE:HB	1.94	0.50
1:D:28:ARG:NH2	1:D:267:GLU:OE2	2.39	0.50
1:D:803:LEU:O	1:D:806:ALA:HB3	2.12	0.50
1:A:112:ARG:HG3	1:A:223:LEU:HD11	1.94	0.49
1:A:451:GLY:HA3	1:A:464:VAL:HB	1.94	0.49
1:C:353:ASN:ND2	3:C:902:NAG:C7	2.75	0.49
1:A:397:VAL:HB	1:A:442:LEU:HD23	1.94	0.49
1:A:460:TRP:NE1	1:A:488:VAL:HG11	2.27	0.49
1:B:642:GLN:OE1	1:B:645:ILE:N	2.34	0.49
1:A:742:LEU:C	1:A:745:PRO:HD2	2.38	0.49
1:C:60:PHE:CE2	1:C:86:PHE:HB3	2.48	0.49
1:A:75:TYR:CE2	1:A:96:THR:HG21	2.48	0.49
1:B:436:CYS:SG	1:B:745:PRO:HB2	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:ILE:HG13	1:B:608:PHE:CZ	2.47	0.49
1:D:485:ARG:O	1:D:489:ILE:HG13	2.12	0.49
1:A:615:SER:HA	1:B:620:LEU:HD23	1.95	0.49
1:C:742:LEU:C	1:C:745:PRO:HD2	2.38	0.49
1:B:737:PRO:HG2	1:B:740:SER:HB2	1.94	0.49
1:C:375:VAL:HG13	3:C:902:NAG:H61	1.94	0.49
1:A:373:SER:HB3	1:A:376:ASP:HB2	1.95	0.48
1:B:522:ALA:O	1:B:526:TRP:N	2.42	0.48
1:D:402:GLU:O	1:D:405:TYR:N	2.44	0.48
1:C:705:GLU:OE1	1:C:732:TYR:OH	2.19	0.48
1:D:75:TYR:CE2	1:D:96:THR:HG21	2.48	0.48
1:D:297:LEU:HD13	1:D:304:ILE:HD13	1.94	0.48
1:D:765:LYS:O	1:D:769:ASP:HB2	2.13	0.48
1:D:245:ILE:HD13	1:D:356:ILE:HG12	1.96	0.48
1:A:502:ILE:HG12	1:A:703:LEU:HD23	1.96	0.48
1:B:297:LEU:HD13	1:B:304:ILE:HD13	1.95	0.48
1:B:525:ILE:HG12	1:C:789:LEU:HB3	1.95	0.48
1:C:8:ASN:HB2	1:C:39:PHE:HA	1.96	0.48
1:C:513:GLY:N	1:C:790:SER:O	2.46	0.48
1:D:450:TYR:O	1:D:463:MET:N	2.47	0.48
1:A:453:ARG:HB2	1:A:460:TRP:CE2	2.48	0.48
1:D:711:TYR:O	1:D:715:ARG:HG2	2.14	0.48
1:B:512:PRO:HB3	1:B:516:SER:HB3	1.95	0.47
1:A:640:SER:HB2	1:A:670:MET:HG2	1.96	0.47
1:B:114:ASP:CG	1:B:116:LYS:HZ2	2.21	0.47
1:C:99:PHE:HA	1:C:112:ARG:HD2	1.96	0.47
1:C:795:VAL:HA	1:C:798:ILE:HG22	1.94	0.47
1:A:799:LEU:HD22	1:D:608:PHE:CZ	2.49	0.47
1:C:525:ILE:HG23	1:C:529:ILE:HB	1.96	0.47
2:D:901:KAI:HD12	2:D:901:KAI:HD2	1.68	0.47
1:D:796:PHE:O	1:D:800:VAL:HG23	2.15	0.47
1:C:177:SER:O	1:C:181:ASP:HB2	2.14	0.47
1:D:742:LEU:O	1:D:745:PRO:HD2	2.15	0.47
2:A:901:KAI:HD12	2:A:901:KAI:HD2	1.64	0.47
1:C:792:VAL:O	1:C:795:VAL:HG12	2.14	0.47
1:A:467:LEU:HG	1:A:737:PRO:HD3	1.97	0.46
1:B:520:PRO:HA	1:B:619:ASN:ND2	2.24	0.46
1:D:763:LYS:O	1:D:767:TRP:HB2	2.15	0.46
1:B:607:PHE:O	1:B:611:ILE:HG12	2.14	0.46
1:A:133:TYR:OH	1:A:193:ASP:OD2	2.26	0.46
1:A:637:GLU:O	1:A:640:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:HD22	1:D:608:PHE:CE1	2.50	0.46
1:D:378:MET:HE3	1:D:378:MET:HB2	1.80	0.46
1:D:113:PRO:HA	1:D:351:ARG:HB2	1.97	0.46
1:A:485:ARG:O	1:A:489:ILE:HG13	2.15	0.46
1:B:96:THR:HA	1:B:97:PRO:HD3	1.77	0.46
1:B:445:VAL:HG13	1:B:448:GLY:HA2	1.98	0.46
1:C:485:ARG:O	1:C:489:ILE:HG13	2.16	0.46
1:A:636:ALA:HA	1:A:639:LEU:CB	2.45	0.46
1:B:485:ARG:O	1:B:489:ILE:HG13	2.16	0.46
1:C:650:LEU:HD13	2:C:901:KAI:HD23	1.97	0.46
1:D:792:VAL:HA	1:D:795:VAL:HG12	1.98	0.46
1:A:291:THR:HG22	1:A:295:ARG:HH12	1.81	0.46
1:B:75:TYR:CE2	1:B:96:THR:HG21	2.50	0.46
1:B:227:ASP:OD2	1:B:277:LYS:HA	2.16	0.46
1:B:756:GLN:HE21	1:B:758:VAL:HG21	1.81	0.46
1:C:502:ILE:HG12	1:C:703:LEU:HD23	1.98	0.46
1:C:529:ILE:HG12	1:C:608:PHE:HZ	1.79	0.46
1:A:297:LEU:HD13	1:A:304:ILE:HG12	1.98	0.45
1:A:635:SER:O	1:A:639:LEU:N	2.49	0.45
1:B:642:GLN:CD	1:B:645:ILE:H	2.23	0.45
1:D:151:ALA:HA	1:D:156:TRP:HB2	1.97	0.45
1:A:75:TYR:HE2	1:A:96:THR:HG21	1.81	0.45
1:B:175:TYR:O	1:B:178:LEU:HG	2.17	0.45
1:D:654:SER:N	2:D:901:KAI:OD2	2.49	0.45
1:C:234:GLN:NE2	1:C:363:THR:O	2.43	0.45
2:B:901:KAI:HD2	2:B:901:KAI:HD12	1.66	0.45
1:A:402:GLU:O	1:A:405:TYR:N	2.50	0.45
1:B:135:TYR:HA	1:B:193:ASP:O	2.17	0.45
1:A:212:HIS:CD2	1:A:236:GLY:HA3	2.52	0.45
1:A:705:GLU:OE1	1:A:732:TYR:OH	2.19	0.45
1:C:651:ASP:O	1:C:656:LYS:NZ	2.39	0.45
1:A:139:ARG:NH2	1:A:193:ASP:OD1	2.47	0.45
1:A:513:GLY:HA3	1:A:790:SER:HB2	1.99	0.45
1:B:611:ILE:HD13	1:C:616:TYR:CE2	2.52	0.45
1:A:498:LEU:HB3	1:A:707:THR:HG23	1.99	0.44
1:A:763:LYS:O	1:A:767:TRP:HB2	2.17	0.44
1:B:292:GLU:HG3	1:B:336:VAL:HG11	1.98	0.44
1:A:476:ILE:HG12	1:A:734:ILE:HG23	1.99	0.44
1:A:636:ALA:O	1:A:640:SER:N	2.51	0.44
1:C:514:VAL:N	1:C:794:GLY:HA3	2.31	0.44
1:D:60:PHE:CE2	1:D:86:PHE:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:GLN:HG3	1:D:260:TRP:HZ2	1.82	0.44
1:A:87:CYS:SG	1:A:94:PHE:HB2	2.58	0.44
1:B:171:LYS:NZ	1:B:201:ASP:OD2	2.50	0.44
1:C:458:LYS:NZ	1:D:155:LYS:HD3	2.33	0.44
1:D:96:THR:HA	1:D:97:PRO:HD3	1.76	0.44
1:D:291:THR:HG22	1:D:295:ARG:HH12	1.82	0.44
1:D:381:THR:HG22	1:D:382:LEU:N	2.27	0.44
1:A:642:GLN:HE22	1:A:645:ILE:H	1.66	0.44
1:B:403:SER:HA	1:B:404:PRO:HA	1.77	0.44
1:C:789:LEU:O	1:C:791:ASN:N	2.51	0.44
1:D:163:VAL:HA	1:D:166:ILE:HD13	2.00	0.44
1:A:799:LEU:HD13	1:D:608:PHE:CG	2.53	0.44
1:B:113:PRO:HA	1:B:351:ARG:HB2	1.98	0.43
1:C:52:ASN:OD1	1:D:85:SER:OG	2.35	0.43
1:C:457:THR:HG22	1:C:459:ILE:HG13	2.00	0.43
1:B:612:ILE:HD13	1:C:792:VAL:HG11	2.00	0.43
1:C:742:LEU:O	1:C:745:PRO:HD2	2.18	0.43
1:C:105:HIS:HA	1:C:106:PRO:HD3	1.90	0.43
1:D:169:ASP:OD2	1:D:170:LYS:HG2	2.17	0.43
1:B:467:LEU:HG	1:B:737:PRO:HD3	2.00	0.43
1:A:8:ASN:HB2	1:A:39:PHE:HA	2.00	0.43
1:A:111:MET:HE3	1:A:286:ALA:HA	2.01	0.43
1:B:31:MET:HE1	1:B:41:LEU:HB2	1.99	0.43
1:B:75:TYR:HE2	1:B:96:THR:HG21	1.84	0.43
1:D:708:MET:HE2	2:D:901:KAI:HD12	2.00	0.43
1:A:60:PHE:CE2	1:A:86:PHE:HB3	2.54	0.43
1:A:752:LYS:NZ	1:A:756:GLN:OE1	2.52	0.43
1:C:96:THR:HA	1:C:97:PRO:HD3	1.77	0.43
1:D:124:GLU:OE2	1:D:154:LYS:NZ	2.45	0.43
1:B:511:LYS:HA	1:B:512:PRO:HD3	1.89	0.43
2:C:901:KAI:HD12	2:C:901:KAI:HD2	1.68	0.43
1:A:517:PHE:CE2	1:A:521:LEU:HD11	2.53	0.43
1:D:176:ARG:HD3	1:D:176:ARG:C	2.44	0.43
1:D:403:SER:HA	1:D:404:PRO:HA	1.74	0.43
1:D:744:THR:OG1	1:D:745:PRO:HD3	2.18	0.43
1:A:527:MET:HE2	1:A:527:MET:HB3	1.92	0.43
1:B:124:GLU:OE2	1:B:154:LYS:NZ	2.50	0.43
1:C:257:ILE:HA	1:C:260:TRP:HB3	2.00	0.43
1:D:329:ARG:HA	1:D:332:LYS:HG2	2.00	0.43
1:A:99:PHE:HA	1:A:100:PRO:HD3	1.92	0.42
1:A:304:ILE:H	1:A:304:ILE:HG13	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LEU:HD22	1:A:526:TRP:HZ2	1.83	0.42
1:B:464:VAL:HG13	1:B:489:ILE:HG12	2.00	0.42
1:B:525:ILE:HD11	1:C:787:LEU:HD21	2.00	0.42
1:C:133:TYR:CD1	1:C:144:LEU:HD13	2.53	0.42
1:C:179:PHE:CD1	1:C:209:ILE:HG13	2.54	0.42
1:A:234:GLN:NE2	1:A:363:THR:O	2.50	0.42
1:B:60:PHE:HE2	1:B:90:LEU:HD12	1.83	0.42
1:B:507:PRO:HG3	1:B:632:PRO:HG3	2.01	0.42
1:D:75:TYR:HE2	1:D:96:THR:HG21	1.83	0.42
1:D:128:TRP:CE2	1:D:189:ARG:HD3	2.53	0.42
1:D:358:ILE:HD11	1:D:372:TRP:HB2	2.00	0.42
1:D:447:ASP:OD2	1:D:462:GLY:HA2	2.18	0.42
1:D:623:PHE:HD1	1:D:623:PHE:HA	1.71	0.42
1:B:28:ARG:NH2	1:B:267:GLU:OE2	2.39	0.42
1:A:809:VAL:HA	1:A:812:ILE:HG12	2.01	0.42
1:A:490:ASP:OD2	1:A:738:LYS:HA	2.20	0.42
1:B:111:MET:HE3	1:B:286:ALA:HA	2.01	0.42
1:B:517:PHE:O	1:B:520:PRO:HD2	2.20	0.42
1:C:75:TYR:HE2	1:C:96:THR:HG21	1.85	0.42
1:C:291:THR:HG22	1:C:295:ARG:HH12	1.85	0.42
1:A:403:SER:HA	1:A:404:PRO:HA	1.75	0.42
1:B:100:PRO:HD3	1:B:112:ARG:HD2	2.01	0.42
1:C:12:ILE:HD13	1:C:41:LEU:HD23	2.00	0.42
1:C:321:TRP:H	1:C:321:TRP:HD1	1.67	0.42
1:C:374:GLU:OE2	3:C:902:NAG:O6	2.31	0.42
1:C:708:MET:O	1:C:712:ILE:HG12	2.19	0.42
1:C:529:ILE:HD11	1:C:612:ILE:HG13	2.01	0.42
1:C:539:VAL:HG13	1:D:807:MET:SD	2.60	0.42
1:B:171:LYS:HE2	1:B:175:TYR:CE1	2.54	0.42
1:B:483:LEU:N	1:C:755:GLU:OE2	2.36	0.42
1:B:518:LEU:HB3	1:B:526:TRP:HE1	1.84	0.42
1:D:526:TRP:O	1:D:529:ILE:HG22	2.20	0.42
1:A:193:ASP:CA	1:A:221:ALA:HB3	2.50	0.42
1:A:481:ILE:HG23	1:A:491:PHE:CD2	2.55	0.42
1:A:650:LEU:HD23	1:A:683:VAL:HG23	2.02	0.41
1:B:402:GLU:O	1:B:405:TYR:N	2.51	0.41
1:B:395:VAL:HG13	1:B:473:ASP:HB2	2.02	0.41
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.55	0.41
1:D:34:PHE:CZ	1:D:288:GLN:HB2	2.55	0.41
1:A:295:ARG:HG2	1:A:299:LYS:HE3	2.02	0.41
1:B:523:TYR:HA	1:B:526:TRP:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:VAL:HG13	1:C:448:GLY:HA2	2.02	0.41
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.56	0.41
1:A:101:THR:OG1	1:A:350:LYS:NZ	2.53	0.41
1:C:420:ARG:NH1	1:C:421:TYR:OH	2.53	0.41
1:A:125:TYR:CE2	1:A:380:VAL:HG11	2.56	0.41
1:B:604:VAL:HG12	1:C:799:LEU:HD12	2.03	0.41
1:D:111:MET:HE3	1:D:286:ALA:HA	2.02	0.41
1:D:113:PRO:HD2	1:D:223:LEU:HD11	2.03	0.41
1:D:114:ASP:OD1	1:D:116:LYS:NZ	2.52	0.41
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.03	0.41
1:D:508:GLN:C	1:D:510:SER:H	2.29	0.41
1:D:607:PHE:O	1:D:611:ILE:HG12	2.21	0.41
1:B:457:THR:HG23	1:B:459:ILE:H	1.86	0.41
1:C:22:GLN:NE2	1:C:270:GLY:O	2.33	0.41
1:C:367:ARG:HA	1:C:367:ARG:CZ	2.50	0.41
1:D:183:GLU:OE1	1:D:211:LYS:NZ	2.49	0.41
1:D:259:ARG:O	1:D:263:LEU:HG	2.21	0.41
1:B:702:TYR:HE2	1:B:704:LEU:HD22	1.86	0.41
1:C:716:LYS:HA	1:C:718:CYS:SG	2.61	0.41
1:D:33:GLN:HG2	1:D:284:TYR:OH	2.21	0.41
1:D:375:VAL:O	1:D:377:LYS:HG3	2.20	0.41
1:C:522:ALA:O	1:C:524:GLU:N	2.54	0.40
1:B:72:PHE:CZ	1:B:283:THR:HG23	2.57	0.40
1:C:31:MET:HE1	1:C:41:LEU:HB2	2.02	0.40
1:A:451:GLY:HA2	1:A:461:ASN:O	2.21	0.40
1:C:494:PRO:HA	1:C:732:TYR:O	2.21	0.40
1:D:119:LEU:O	1:D:123:ILE:HG13	2.22	0.40
1:D:597:SER:O	1:D:600:ILE:HG12	2.22	0.40
1:A:526:TRP:HA	1:A:529:ILE:HG22	2.02	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	708/824 (86%)	694 (98%)	14 (2%)	0	100	100
1	B	738/824 (90%)	731 (99%)	7 (1%)	0	100	100
1	C	732/824 (89%)	719 (98%)	13 (2%)	0	100	100
1	D	739/824 (90%)	725 (98%)	14 (2%)	0	100	100
All	All	2917/3296 (88%)	2869 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	549/701 (78%)	539 (98%)	10 (2%)	51	69
1	B	586/701 (84%)	572 (98%)	14 (2%)	43	64
1	C	573/701 (82%)	562 (98%)	11 (2%)	50	68
1	D	571/701 (82%)	556 (97%)	15 (3%)	40	63
All	All	2279/2804 (81%)	2229 (98%)	50 (2%)	45	66

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	205	GLN
1	A	319	VAL
1	A	335	GLN
1	A	456	ASP
1	A	498	LEU
1	A	504	ILE
1	A	633	ILE
1	A	669	LYS
1	A	789	LEU
1	B	77	LYS
1	B	110	GLN
1	B	170	LYS

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Mol	Chain	Res	Type
1	B	174	THR
1	B	184	LEU
1	B	192	LEU
1	B	233	ILE
1	B	239	GLU
1	B	267	GLU
1	B	319	VAL
1	B	391	GLU
1	B	498	LEU
1	B	511	LYS
1	B	814	PHE
1	C	110	GLN
1	C	178	LEU
1	C	180	GLN
1	C	319	VAL
1	C	321	TRP
1	C	367	ARG
1	C	498	LEU
1	C	529	ILE
1	C	789	LEU
1	C	799	LEU
1	C	812	ILE
1	D	77	LYS
1	D	110	GLN
1	D	167	ASN
1	D	192	LEU
1	D	233	ILE
1	D	319	VAL
1	D	378	MET
1	D	394	THR
1	D	498	LEU
1	D	525	ILE
1	D	529	ILE
1	D	612	ILE
1	D	623	PHE
1	D	773	CYS
1	D	799	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN

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Mol	Chain	Res	Type
1	A	205	GLN
1	B	200	ASN
1	B	335	GLN
1	B	342	ASN
1	B	412	HIS
1	C	412	HIS
1	D	162	ASN
1	D	167	ASN
1	D	205	GLN
1	D	412	HIS

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](#)

7 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	KAI	A	901	-	13,15,15	1.04	0	12,21,21	1.07	1 (8%)
2	KAI	D	901	-	13,15,15	1.06	0	12,21,21	1.13	1 (8%)
2	KAI	C	901	-	13,15,15	1.01	0	12,21,21	1.08	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KAI	B	901	-	13,15,15	1.05	0	12,21,21	1.10	1 (8%)
3	NAG	A	902	1	14,14,15	1.24	2 (14%)	17,19,21	2.52	6 (35%)
3	NAG	B	902	1	14,14,15	0.51	0	17,19,21	0.93	0
3	NAG	C	902	1	14,14,15	0.30	0	17,19,21	1.47	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAI	A	901	-	-	4/12/25/25	0/1/1/1
2	KAI	D	901	-	-	0/12/25/25	0/1/1/1
2	KAI	C	901	-	-	0/12/25/25	0/1/1/1
2	KAI	B	901	-	-	1/12/25/25	0/1/1/1
3	NAG	A	902	1	-	2/6/23/26	0/1/1/1
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
3	NAG	C	902	1	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	NAG	O5-C1	-2.39	1.39	1.43
3	A	902	NAG	O4-C4	2.18	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	NAG	C1-O5-C5	5.73	119.87	112.19
3	A	902	NAG	O5-C1-C2	5.08	119.16	111.29
3	C	902	NAG	C2-N2-C7	-4.25	117.21	122.90
3	A	902	NAG	O5-C5-C4	3.40	119.10	110.83
3	A	902	NAG	C6-C5-C4	-2.80	106.15	113.02
3	A	902	NAG	C4-C3-C2	-2.53	107.31	111.02
2	C	901	KAI	CB-CA-C	-2.46	109.04	113.98
3	C	902	NAG	C4-C3-C2	-2.36	107.56	111.02
3	A	902	NAG	O4-C4-C3	2.21	115.58	110.38
2	D	901	KAI	CB-CA-C	-2.20	109.57	113.98
2	B	901	KAI	CB-CA-C	-2.18	109.60	113.98
2	A	901	KAI	CB-CA-C	-2.08	109.81	113.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	NAG	C8-C7-N2-C2
3	C	902	NAG	O7-C7-N2-C2
3	A	902	NAG	C8-C7-N2-C2
3	A	902	NAG	O7-C7-N2-C2
3	C	902	NAG	C1-C2-N2-C7
2	A	901	KAI	OXT-C-CA-CB
2	A	901	KAI	OXT-C-CA-N
2	A	901	KAI	O-C-CA-CB
2	A	901	KAI	O-C-CA-N
2	B	901	KAI	CA-CB-CB1-CG1

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	KAI	1	0
2	D	901	KAI	3	0
2	C	901	KAI	2	0
2	B	901	KAI	2	0
3	C	902	NAG	3	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, 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	721/824 (87%)	-0.23	11 (1%) 72 44	152, 223, 280, 321	0
1	B	746/824 (90%)	-0.14	19 (2%) 58 33	144, 216, 276, 314	0
1	C	744/824 (90%)	-0.12	27 (3%) 46 25	150, 223, 283, 349	0
1	D	749/824 (90%)	-0.04	29 (3%) 43 23	154, 223, 283, 329	0
All	All	2960/3296 (89%)	-0.13	86 (2%) 53 30	144, 221, 281, 349	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	CYS	9.6
1	C	634	GLU	8.0
1	C	635	SER	7.5
1	C	760	ASP	6.0
1	D	136	ASP	5.8
1	D	517	PHE	5.5
1	C	335	GLN	5.4
1	D	395	VAL	5.2
1	D	210	GLY	5.2
1	D	791	ASN	4.6
1	C	638	ASP	4.5
1	A	158	VAL	4.2
1	D	192	LEU	4.2
1	D	777	ASP	4.1
1	C	792	VAL	3.6
1	D	523	TYR	3.6
1	D	131	PHE	3.6
1	C	636	ALA	3.5
1	D	133	TYR	3.5
1	A	243	PHE	3.5
1	C	791	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	725	GLY	3.4
1	D	671	TRP	3.4
1	C	641	LYS	3.3
1	B	540	LEU	3.3
1	D	518	LEU	3.3
1	B	728	ASP	3.2
1	C	788	SER	3.2
1	C	223	LEU	3.2
1	C	783	LYS	3.1
1	D	134	LEU	3.1
1	B	633	ILE	2.9
1	B	153	GLU	2.9
1	B	478	PRO	2.9
1	B	726	ASN	2.9
1	C	243	PHE	2.8
1	C	141	LEU	2.8
1	D	674	MET	2.8
1	A	761	LYS	2.7
1	D	604	VAL	2.7
1	A	686	THR	2.7
1	D	193	ASP	2.6
1	D	769	ASP	2.6
1	C	49	GLU	2.6
1	D	478	PRO	2.6
1	C	758	VAL	2.6
1	C	222	ASN	2.6
1	C	654	SER	2.5
1	B	310	ALA	2.5
1	D	458	LYS	2.5
1	B	12	ILE	2.5
1	C	757	GLY	2.4
1	A	529	ILE	2.4
1	D	218	TYR	2.4
1	B	729	SER	2.4
1	A	208	THR	2.4
1	C	92	VAL	2.4
1	B	442	LEU	2.4
1	B	769	ASP	2.4
1	B	70	ALA	2.4
1	B	696	SER	2.3
1	A	223	LEU	2.3
1	D	650	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLY	2.3
1	A	627	GLU	2.3
1	D	792	VAL	2.3
1	B	667	PHE	2.2
1	D	607	PHE	2.2
1	D	135	TYR	2.2
1	A	762	LEU	2.2
1	D	657	GLU	2.2
1	C	342	ASN	2.2
1	C	138	ASP	2.2
1	D	319	VAL	2.2
1	C	224	GLY	2.2
1	C	194	CYS	2.1
1	D	429	ALA	2.1
1	C	93	SER	2.1
1	C	220	ILE	2.1
1	C	344	LYS	2.1
1	A	339	LEU	2.1
1	D	686	THR	2.1
1	A	379	VAL	2.1
1	B	813	GLU	2.0
1	B	598	ALA	2.0
1	B	230	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	902	14/15	0.39	0.12	310,368,455,556	0
2	KAI	A	901	15/15	0.68	0.14	171,255,312,320	0
2	KAI	C	901	15/15	0.83	0.18	167,209,275,295	0
2	KAI	B	901	15/15	0.93	0.14	116,167,282,304	0
3	NAG	A	902	14/15	0.94	0.09	143,200,293,296	0
3	NAG	C	902	14/15	0.95	0.07	113,199,304,331	0
2	KAI	D	901	15/15	0.98	0.10	137,198,325,346	0

6.5 Other polymers [i](#)

There are no such residues in this entry.