



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 09:27 AM EDT

PDB ID : 2F36
Title : Crystal Structure of the GluR5 Ligand Binding Core Dimer with Glutamate
At 2.1 Angstroms Resolution
Authors : Mayer, M.L.
Deposited on : 2005-11-18
Resolution : 2.11 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 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 : 2.23.2
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) : 2.23.2

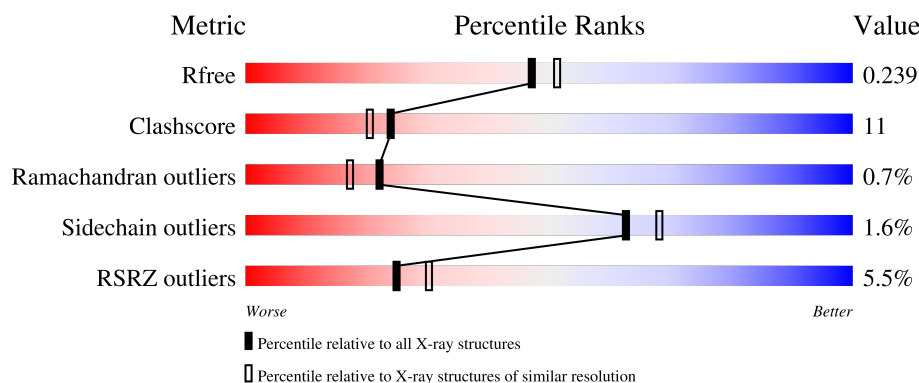
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	258	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	B	258	<div> <div>3%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
1	C	258	<div> <div>3%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	D	258	<div> <div>12%</div> <div>68%</div> <div>26%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8567 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.

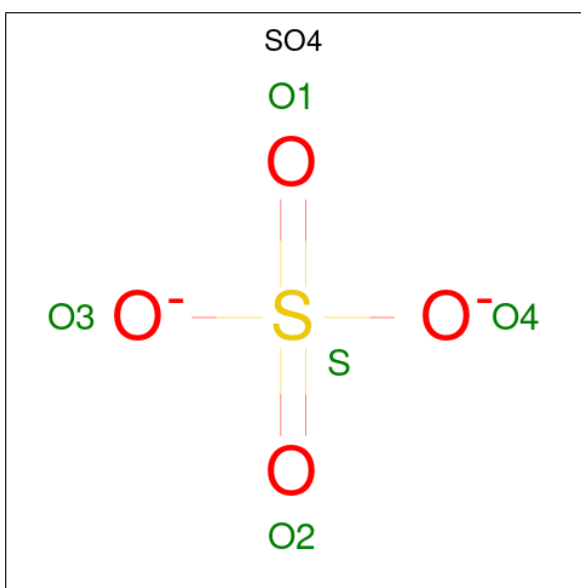
- Molecule 1 is a protein called GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	8	0	0
			2020	1289	334	385	12			
1	B	248	Total	C	N	O	S	16	5	0
			2030	1295	340	384	11			
1	C	254	Total	C	N	O	S	32	0	0
			2020	1289	334	385	12			
1	D	248	Total	C	N	O	S	59	1	0
			1993	1275	329	378	11			

There are 20 discrepancies between the modelled and reference sequences:

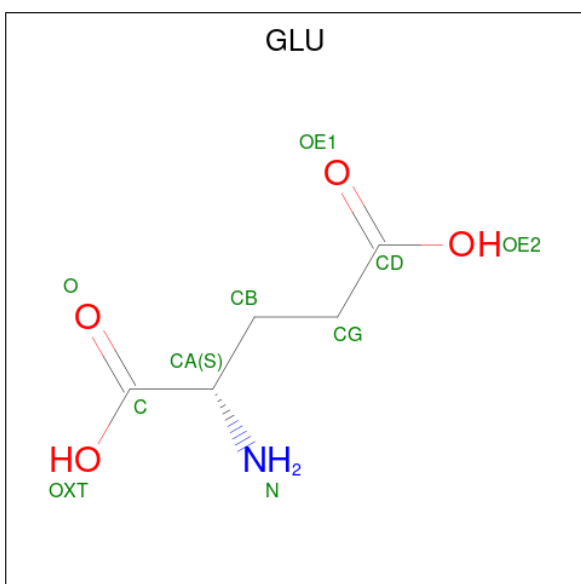
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P22756
A	2	SER	-	cloning artifact	UNP P22756
A	117	GLY	-	linker	UNP P22756
A	118	THR	-	linker	UNP P22756
A	258	SER	GLU	engineered mutation	UNP P22756
B	1	GLY	-	cloning artifact	UNP P22756
B	2	SER	-	cloning artifact	UNP P22756
B	117	GLY	-	linker	UNP P22756
B	118	THR	-	linker	UNP P22756
B	258	SER	GLU	engineered mutation	UNP P22756
C	1	GLY	-	cloning artifact	UNP P22756
C	2	SER	-	cloning artifact	UNP P22756
C	117	GLY	-	linker	UNP P22756
C	118	THR	-	linker	UNP P22756
C	258	SER	GLU	engineered mutation	UNP P22756
D	1	GLY	-	cloning artifact	UNP P22756
D	2	SER	-	cloning artifact	UNP P22756
D	117	GLY	-	linker	UNP P22756
D	118	THR	-	linker	UNP P22756
D	258	SER	GLU	engineered mutation	UNP P22756

- Molecule 2 is SULFATE ION (three-letter code: 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	1
			10	8	2		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	A	1	Total	C	N	O	0	0
			10	5	1	4		

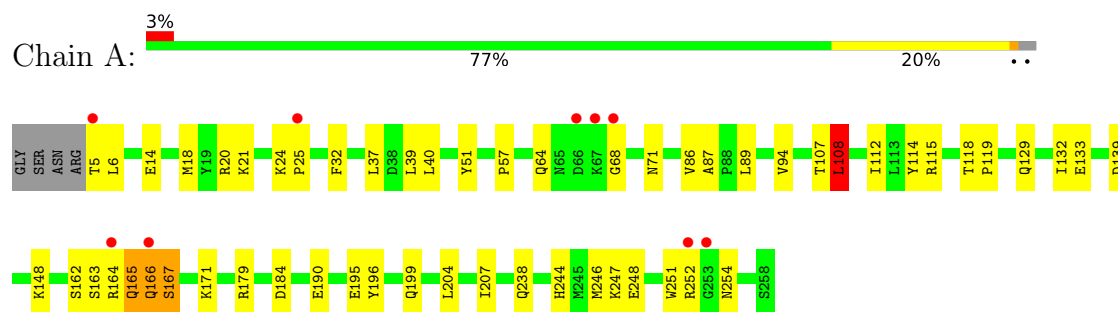
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	0
			150	150		
4	B	153	Total	O	0	0
			153	153		
4	C	92	Total	O	0	0
			92	92		
4	D	44	Total	O	0	0
			44	44		

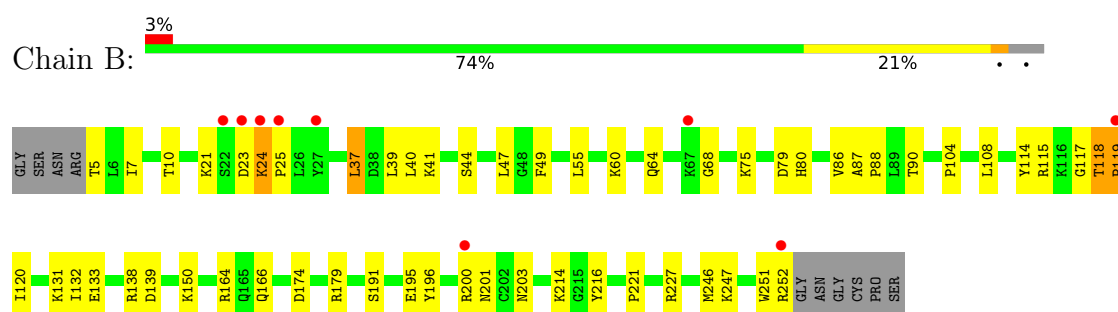
3 Residue-property plots [i](#)

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.

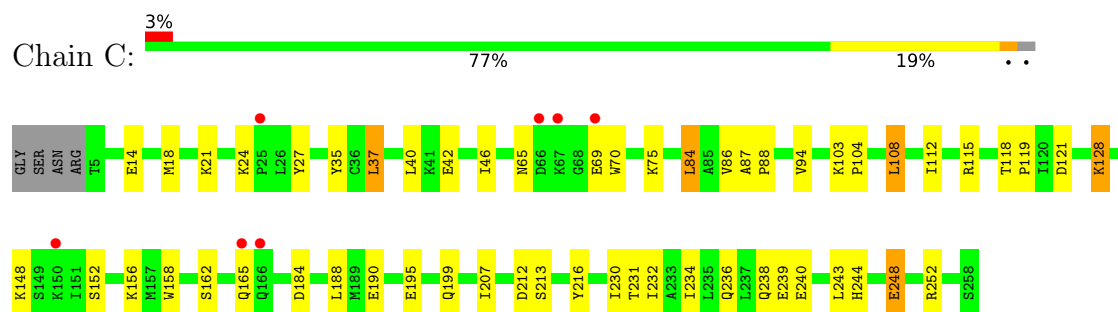
• Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 1



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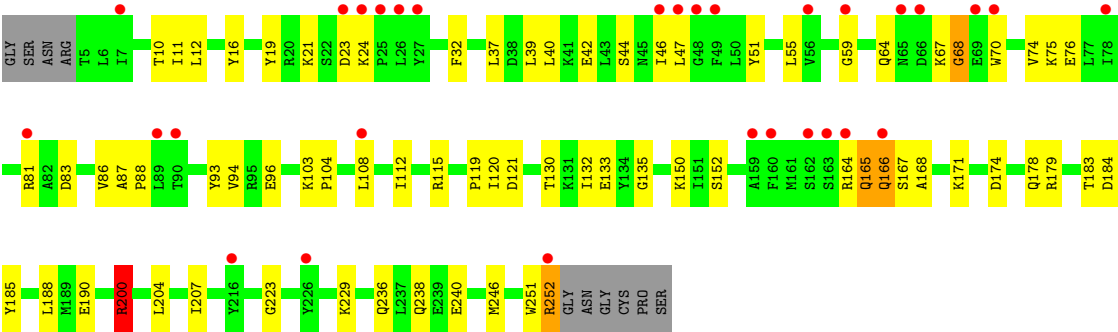


• Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 1



• Molecule 1: GLUTAMATE RECEPTOR, IONOTROPIC KAINATE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.69Å 73.78Å 115.92Å 90.00° 99.74° 90.00°	Depositor
Resolution (Å)	29.87 – 2.11 29.86 – 2.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.87-2.11) 99.2 (29.86-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.241 0.186 , 0.239	Depositor DCC
R_{free} test set	6016 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.6	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	0.95	EDS
Total number of atoms	8567	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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	0.84	2/2059 (0.1%)	0.93	4/2776 (0.1%)
1	B	0.95	2/2069 (0.1%)	1.03	6/2789 (0.2%)
1	C	0.96	3/2059 (0.1%)	0.94	6/2776 (0.2%)
1	D	1.24	9/2031 (0.4%)	0.95	10/2739 (0.4%)
All	All	1.01	16/8218 (0.2%)	0.96	26/11080 (0.2%)

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	D	1	0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	152	SER	CB-OG	36.31	1.89	1.42
1	C	27	TYR	CA-CB	21.47	2.01	1.53
1	D	24	LYS	CA-CB	20.43	1.98	1.53
1	B	23	ASP	CA-CB	-17.39	1.15	1.53
1	D	164	ARG	CA-CB	-16.62	1.17	1.53
1	D	83	ASP	CB-CG	14.37	1.81	1.51
1	C	248	GLU	CG-CD	-13.63	1.31	1.51
1	C	21	LYS	CA-CB	-13.05	1.25	1.53
1	D	200	ARG	CG-CD	7.60	1.71	1.51
1	A	166	GLN	CG-CD	7.14	1.67	1.51
1	D	171	LYS	CA-CB	-6.95	1.38	1.53
1	D	150	LYS	CG-CD	6.88	1.75	1.52
1	A	167	SER	CB-OG	6.00	1.50	1.42
1	D	21	LYS	CA-CB	-5.58	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	75	LYS	CA-CB	-5.16	1.42	1.53
1	B	21	LYS	CB-CG	-5.00	1.39	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ASP	N-CA-CB	15.46	138.42	110.60
1	D	75	LYS	N-CA-CB	13.58	135.04	110.60
1	D	164	ARG	N-CA-CB	12.95	133.92	110.60
1	B	23	ASP	CA-CB-CG	-10.54	90.21	113.40
1	C	27	TYR	CB-CA-C	-9.01	92.39	110.40
1	A	37	LEU	CA-CB-CG	-8.71	95.27	115.30
1	C	27	TYR	N-CA-CB	-8.40	95.48	110.60
1	B	227	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	D	83	ASP	CB-CG-OD2	7.83	125.35	118.30
1	B	227	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	24	LYS	N-CA-CB	-7.57	96.97	110.60
1	C	37	LEU	CA-CB-CG	-7.56	97.90	115.30
1	D	83	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	B	37	LEU	CA-CB-CG	-7.11	98.94	115.30
1	C	24	LYS	N-CA-CB	-6.85	98.27	110.60
1	D	188	LEU	CA-CB-CG	6.40	130.02	115.30
1	D	166	GLN	N-CA-CB	6.18	121.73	110.60
1	C	84	LEU	CA-CB-CG	6.06	129.23	115.30
1	D	75	LYS	CA-CB-CG	5.86	126.29	113.40
1	D	152	SER	CA-CB-OG	-5.60	96.07	111.20
1	A	108	LEU	CB-CG-CD1	5.47	120.31	111.00
1	A	37	LEU	CB-CG-CD1	5.46	120.29	111.00
1	D	74	VAL	CB-CA-C	-5.37	101.19	111.40
1	D	74	VAL	CA-CB-CG2	-5.09	103.26	110.90
1	C	21	LYS	CB-CA-C	5.08	120.55	110.40
1	A	167	SER	CA-CB-OG	-5.01	97.67	111.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	164	ARG	CA

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	2020	0	2036	44	0
1	B	2030	0	2049	53	0
1	C	2020	0	2036	38	1
1	D	1993	0	2016	52	1
2	A	5	0	0	1	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	40	0	20	1	0
4	A	150	0	0	7	0
4	B	153	0	0	7	0
4	C	92	0	0	5	0
4	D	44	0	0	2	0
All	All	8567	0	8157	177	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (177) 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:200:ARG:NH2	1:B:252:ARG:HG3	1.28	1.46
1:D:200:ARG:HG3	1:D:252:ARG:HH22	1.09	1.12
1:D:200:ARG:CG	1:D:252:ARG:NH2	2.15	1.09
1:B:118:THR:HB	1:B:119:PRO:HD3	1.34	1.07
1:B:200:ARG:NH2	1:B:252:ARG:CG	2.21	1.03
1:D:200:ARG:HG3	1:D:252:ARG:NH2	1.72	1.03
1:B:118:THR:HB	1:B:119:PRO:CD	1.90	1.02
1:D:200:ARG:CG	1:D:252:ARG:HH22	1.72	1.00
1:B:200:ARG:HH22	1:B:252:ARG:HG3	1.16	0.96
1:A:133:GLU:OE1	1:A:179:ARG:NH2	1.97	0.96
1:D:174:ASP:O	1:D:178:GLN:HG2	1.68	0.93
1:B:200:ARG:HH21	1:B:252:ARG:HG3	1.30	0.93
1:B:114:TYR:CE2	1:B:118:THR:HG21	2.03	0.92
1:A:115:ARG:HD3	4:A:644:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:HD12	1:D:190:GLU:HB3	1.53	0.90
1:D:42:GLU:O	1:D:46:ILE:HG12	1.76	0.86
1:B:5:THR:HG23	4:B:711:HOH:O	1.75	0.86
1:B:118:THR:CB	1:B:119:PRO:CD	2.55	0.84
1:B:138:ARG:NH1	1:B:166:GLN:OE1	2.13	0.81
1:C:115:ARG:HD3	4:C:675:HOH:O	1.80	0.81
1:C:195:GLU:O	1:C:199:GLN:HG2	1.80	0.80
1:D:10:THR:HG23	1:D:55:LEU:HD23	1.63	0.80
1:C:121:ASP:OD1	4:C:670:HOH:O	2.03	0.76
1:D:115:ARG:NH1	1:D:184:ASP:OD2	2.18	0.76
1:C:238:GLN:HG2	4:D:642:HOH:O	1.85	0.75
1:A:162:SER:O	1:A:165:GLN:HG3	1.86	0.74
1:B:115:ARG:HB3	1:B:115:ARG:HH11	1.53	0.74
1:C:118:THR:HB	1:C:119:PRO:HD2	1.70	0.73
1:A:165:GLN:OE1	1:A:166:GLN:HG3	1.87	0.73
1:B:80[A]:HIS:HA	4:B:741:HOH:O	1.88	0.72
1:C:158:TRP:O	1:C:162:SER:HB3	1.90	0.69
1:A:24:LYS:HB3	1:A:25:PRO:HD2	1.76	0.67
1:C:213:SER:H	1:D:238[B]:GLN:NE2	1.91	0.67
1:D:251:TRP:C	1:D:252:ARG:HD2	2.14	0.66
1:D:200:ARG:HG2	1:D:252:ARG:NH2	2.09	0.66
1:D:236:GLN:O	1:D:240:GLU:HG2	1.98	0.64
1:D:108:LEU:CD1	1:D:190:GLU:HB3	2.26	0.64
1:C:46:ILE:HD11	4:C:626:HOH:O	1.98	0.64
1:C:230:ILE:O	1:C:234:ILE:HG12	1.98	0.64
1:A:254:ASN:HA	1:C:244:HIS:CE1	2.33	0.63
1:C:108:LEU:HD13	1:C:190:GLU:HB3	1.80	0.63
1:C:42:GLU:O	1:C:46:ILE:HG12	1.98	0.63
1:B:150:LYS:HE2	4:B:725:HOH:O	1.99	0.62
1:C:65:ASN:OD1	1:C:69:GLU:HG2	1.99	0.62
1:A:195:GLU:O	1:A:199:GLN:HG2	1.99	0.62
1:A:133:GLU:OE2	1:A:164:ARG:NH2	2.33	0.62
1:B:247:LYS:HD2	1:B:251:TRP:CE3	2.34	0.62
1:B:117:GLY:O	4:B:735:HOH:O	2.16	0.61
1:B:115:ARG:HB3	1:B:115:ARG:NH1	2.16	0.61
1:B:200:ARG:N	1:B:200:ARG:HD2	2.15	0.61
1:A:199:GLN:HG3	4:A:640:HOH:O	1.99	0.61
1:A:5:THR:CG2	4:A:657:HOH:O	2.49	0.61
1:A:167:SER:O	1:A:179:ARG:NH1	2.30	0.60
1:A:5:THR:HG21	4:A:657:HOH:O	1.99	0.60
1:C:128:LYS:HB3	1:C:128:LYS:NZ	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:TYR:CE2	1:B:118:THR:CG2	2.82	0.59
1:B:114:TYR:HE2	1:B:118:THR:CB	2.15	0.59
1:A:248:GLU:O	1:A:252:ARG:HB2	2.04	0.58
1:B:64:GLN:NE2	1:B:68:GLY:HA2	2.19	0.58
1:D:183:THR:HG22	1:D:184:ASP:N	2.18	0.57
1:D:64:GLN:HE21	1:D:68:GLY:C	2.08	0.57
1:C:87:ALA:HB1	1:C:88:PRO:HD2	1.87	0.57
1:A:171:LYS:HE3	4:A:746:HOH:O	2.05	0.56
1:D:238[A]:GLN:NE2	4:D:634:HOH:O	1.83	0.56
1:B:201:ASN:OD1	1:B:203:ASN:HB2	2.06	0.56
1:A:57:PRO:HD2	4:A:674:HOH:O	2.05	0.56
1:D:39:LEU:N	1:D:246:MET:HE1	2.21	0.55
1:D:32:PHE:HB3	1:D:37:LEU:HD11	1.87	0.55
1:C:152:SER:O	1:C:156:LYS:HG3	2.07	0.55
1:C:103:LYS:HG2	1:C:231:THR:HG23	1.88	0.55
1:D:183:THR:CG2	1:D:184:ASP:N	2.70	0.55
1:C:238:GLN:NE2	4:C:694:HOH:O	2.39	0.55
1:B:75:LYS:HE2	1:B:79[A]:ASP:OD2	2.07	0.54
1:B:114:TYR:HE2	1:B:118:THR:HG1	1.56	0.54
1:D:44:SER:OG	1:D:51:TYR:CE2	2.60	0.54
1:D:167:SER:O	1:D:179:ARG:NH1	2.34	0.54
1:C:115:ARG:NH2	1:C:184:ASP:OD1	2.39	0.54
1:D:179:ARG:O	1:D:183:THR:HB	2.08	0.54
1:A:14:GLU:HG2	1:A:196:TYR:CE2	2.43	0.54
1:A:114:TYR:OH	1:A:132:ILE:HD12	2.08	0.54
1:B:221:PRO:HG3	4:B:741:HOH:O	2.07	0.53
1:A:21:LYS:HE3	1:D:120:ILE:HD11	1.90	0.53
1:A:25:PRO:HG2	1:A:25:PRO:O	2.09	0.52
1:B:131:LYS:HE2	4:B:664:HOH:O	2.08	0.52
1:D:132:ILE:HD12	1:D:132:ILE:N	2.24	0.52
1:A:112:ILE:HB	1:A:207:ILE:HB	1.91	0.52
1:C:94:VAL:HG11	1:C:148:LYS:HD2	1.90	0.52
1:A:14:GLU:HG3	1:A:18:MET:SD	2.51	0.51
1:C:70:TRP:O	1:C:75:LYS:HD2	2.09	0.51
1:B:252:ARG:NH1	1:B:252:ARG:HB3	2.25	0.51
1:A:6:LEU:O	1:A:51:TYR:HA	2.11	0.51
1:A:164:ARG:O	1:A:166:GLN:N	2.44	0.51
1:B:10:THR:HG23	1:B:55:LEU:HD23	1.93	0.51
1:B:200:ARG:HH22	1:B:252:ARG:CG	2.05	0.51
1:B:133:GLU:HG3	1:B:164[A]:ARG:HH22	1.76	0.51
1:D:87:ALA:HB1	1:D:88:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:HB3	1:B:252:ARG:CZ	2.41	0.50
1:D:251:TRP:O	1:D:252:ARG:HD2	2.11	0.50
1:D:135:GLY:HA3	1:D:168:ALA:O	2.11	0.50
1:B:214:LYS:HB2	4:B:612:HOH:O	2.11	0.50
1:C:232:ILE:CD1	1:D:96:GLU:HB3	2.42	0.50
1:B:104:PRO:HA	1:B:216:TYR:O	2.12	0.49
1:D:103:LYS:HG3	1:D:104:PRO:HD2	1.93	0.49
1:B:191:SER:O	1:B:195:GLU:HG3	2.11	0.49
1:C:212:ASP:HB2	1:D:238[B]:GLN:HE22	1.78	0.49
1:B:60:LYS:NZ	1:B:139:ASP:OD2	2.38	0.49
1:B:120:ILE:HG12	1:B:132:ILE:CD1	2.43	0.48
1:B:133:GLU:OE1	1:B:179:ARG:NH2	2.46	0.48
1:C:75:LYS:HE3	1:C:75:LYS:HA	1.96	0.47
1:A:21:LYS:HG3	1:D:120:ILE:HD13	1.95	0.47
1:B:39:LEU:HB2	1:B:246:MET:HE1	1.96	0.47
1:A:39:LEU:N	1:A:246:MET:HE1	2.30	0.47
1:D:23:ASP:OD1	1:D:23:ASP:N	2.46	0.47
1:A:21:LYS:HG2	1:D:119:PRO:HG2	1.97	0.47
1:C:84:LEU:HD21	1:C:230:ILE:HD11	1.95	0.47
1:A:87:ALA:O	1:A:89:LEU:N	2.48	0.46
1:D:40:LEU:HD13	1:D:86:VAL:HG21	1.97	0.46
1:B:115:ARG:HH11	1:B:115:ARG:CB	2.27	0.46
1:D:44:SER:HG	1:D:51:TYR:HE2	1.57	0.46
1:B:114:TYR:CE2	1:B:118:THR:CB	2.99	0.46
1:A:21:LYS:CE	1:D:120:ILE:HD11	2.45	0.45
1:A:108:LEU:HD13	1:A:190:GLU:HB3	1.98	0.45
1:D:32:PHE:HB3	1:D:37:LEU:CD1	2.47	0.45
1:B:118:THR:CB	1:B:119:PRO:HD3	2.13	0.45
1:C:238:GLN:HB2	1:C:243:LEU:HD12	1.98	0.44
1:A:24:LYS:HB3	1:A:25:PRO:CD	2.44	0.44
1:A:40:LEU:HD13	1:A:86:VAL:HG21	1.99	0.44
1:B:114:TYR:HE2	1:B:118:THR:OG1	2.00	0.44
1:A:163:SER:OG	1:A:164:ARG:HG3	2.17	0.44
1:C:112:ILE:HB	1:C:207:ILE:HB	2.00	0.44
1:A:25:PRO:O	1:A:25:PRO:CG	2.65	0.44
1:B:7:ILE:HD12	1:B:7:ILE:N	2.33	0.44
1:A:20:ARG:NH2	1:A:32:PHE:O	2.50	0.44
1:A:132:ILE:HD13	1:A:184:ASP:OD2	2.18	0.44
1:D:112:ILE:HB	1:D:207:ILE:HB	2.00	0.44
1:D:32:PHE:C	1:D:37:LEU:HD13	2.37	0.43
1:C:118:THR:HB	1:C:119:PRO:CD	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:THR:O	1:D:130:THR:OG1	2.36	0.43
1:C:239:GLU:OE1	1:D:93:TYR:HE2	2.01	0.43
1:D:70:TRP:HH2	1:D:94:VAL:HG12	1.82	0.43
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.81	0.43
1:D:76:GLU:OE1	1:D:81:ARG:HD2	2.18	0.43
1:B:87:ALA:HB1	1:B:88:PRO:HD2	1.99	0.43
1:B:40:LEU:HD13	1:B:86:VAL:HG21	2.00	0.43
1:A:247:LYS:HD2	1:A:251:TRP:CE3	2.54	0.43
1:D:121:ASP:O	1:D:121:ASP:OD1	2.37	0.43
1:A:244:HIS:NE2	1:A:248:GLU:OE2	2.51	0.43
1:D:16:TYR:CD1	1:D:88:PRO:HG3	2.53	0.43
1:C:236:GLN:O	1:C:240:GLU:HG3	2.19	0.42
1:B:24:LYS:HA	1:B:25:PRO:HD3	1.83	0.42
1:A:94:VAL:HG11	1:A:148:LYS:HE3	2.02	0.42
1:B:196:TYR:O	1:B:200:ARG:HD3	2.19	0.42
1:C:115:ARG:CD	4:C:675:HOH:O	2.52	0.42
1:B:138:ARG:HH12	1:B:166:GLN:CB	2.32	0.42
1:A:129:GLN:OE1	1:A:132:ILE:HG12	2.20	0.42
1:B:118:THR:HB	1:B:119:PRO:HD2	1.93	0.42
1:C:239:GLU:CD	1:D:93:TYR:HE2	2.23	0.42
1:D:44:SER:OG	1:D:51:TYR:CD2	2.72	0.41
3:A:502:GLU:N	1:B:90:THR:HG1	2.19	0.41
1:B:44:SER:HB2	1:B:49:PHE:O	2.20	0.41
1:A:64:GLN:HE21	1:A:68:GLY:HA2	1.86	0.41
1:C:14:GLU:HG3	1:C:18:MET:SD	2.61	0.41
1:C:158:TRP:O	1:C:162:SER:CB	2.66	0.41
1:D:133:GLU:O	1:D:185:TYR:HA	2.21	0.41
1:C:40:LEU:HD13	1:C:86:VAL:HG21	2.03	0.41
1:C:104:PRO:HA	1:C:216:TYR:O	2.20	0.41
1:D:47:LEU:HD22	1:D:229:LYS:HB3	2.03	0.41
1:B:64:GLN:HE21	1:B:68:GLY:HA2	1.85	0.41
1:C:188:LEU:HD22	1:C:188:LEU:N	2.36	0.41
1:A:71:ASN:ND2	1:A:139:ASP:OD2	2.52	0.40
1:A:118:THR:HB	1:A:119:PRO:HD2	2.02	0.40
1:A:238:GLN:NE2	4:A:701:HOH:O	2.37	0.40
1:A:107:THR:OG1	2:A:604:SO4:O3	2.30	0.40
1:C:35:TYR:CD2	1:C:35:TYR:C	2.95	0.40
1:D:11:ILE:HD11	1:D:59:GLY:O	2.21	0.40
1:D:12:LEU:HD11	1:D:19:TYR:CE1	2.56	0.40
1:B:41:LYS:HE3	1:B:41:LYS:HB2	1.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:GLN:NE2	1:D:223:GLY:O[2_646]	2.18	0.02

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	252/258 (98%)	246 (98%)	5 (2%)	1 (0%)	34	32
1	B	251/258 (97%)	243 (97%)	6 (2%)	2 (1%)	19	14
1	C	252/258 (98%)	247 (98%)	5 (2%)	0	100	100
1	D	247/258 (96%)	227 (92%)	16 (6%)	4 (2%)	9	4
All	All	1002/1032 (97%)	963 (96%)	32 (3%)	7 (1%)	22	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	D	165	GLN
1	B	118	THR
1	D	67	LYS
1	B	119	PRO
1	D	166	GLN
1	D	68	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/225 (99%)	220 (99%)	2 (1%)	78	83
1	B	223/225 (99%)	220 (99%)	3 (1%)	69	74
1	C	222/225 (99%)	217 (98%)	5 (2%)	50	53
1	D	219/225 (97%)	215 (98%)	4 (2%)	59	63
All	All	886/900 (98%)	872 (98%)	14 (2%)	62	68

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	204	LEU
1	B	37	LEU
1	B	108	LEU
1	B	174	ASP
1	C	37	LEU
1	C	108	LEU
1	C	128	LYS
1	C	248	GLU
1	C	252	ARG
1	D	165	GLN
1	D	200	ARG
1	D	204	LEU
1	D	252	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	GLN
1	C	64	GLN
1	C	244	HIS
1	D	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
3	GLU	A	504	-	2,9,9	0.84	0	2,11,11	1.10	0
2	SO4	B	601[A]	-	4,4,4	0.19	0	6,6,6	0.40	0
3	GLU	A	501	-	2,9,9	1.10	0	2,11,11	0.25	0
2	SO4	C	603	-	4,4,4	0.12	0	6,6,6	0.21	0
2	SO4	D	602	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	A	604	-	4,4,4	0.16	0	6,6,6	0.30	0
3	GLU	A	503	-	2,9,9	1.51	1 (50%)	2,11,11	0.82	0
2	SO4	B	601[B]	-	4,4,4	0.11	0	6,6,6	0.41	0
3	GLU	A	502	-	2,9,9	0.66	0	2,11,11	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	A	502	-	-	0/3/9/9	-
3	GLU	A	501	-	-	0/3/9/9	-
3	GLU	A	504	-	-	0/3/9/9	-
3	GLU	A	503	-	-	0/3/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	GLU	CA-N	2.12	1.51	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	SO4	1	0
3	A	502	GLU	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, 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	254/258 (98%)	-0.02	9 (3%)	44	50	13, 25, 41, 54	3 (1%)
1	B	248/258 (96%)	-0.03	9 (3%)	42	49	12, 20, 38, 52	4 (1%)
1	C	254/258 (98%)	0.02	7 (2%)	53	59	17, 27, 45, 56	7 (2%)
1	D	248/258 (96%)	0.70	30 (12%)	4	5	22, 38, 53, 61	15 (6%)
All	All	1004/1032 (97%)	0.17	55 (5%)	25	30	12, 27, 48, 61	29 (2%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	ASP	6.4
1	C	165	GLN	5.3
1	B	27	TYR	5.0
1	A	67	LYS	4.9
1	D	252	ARG	4.2
1	C	25	PRO	4.1
1	B	25	PRO	3.8
1	A	66	ASP	3.8
1	B	67	LYS	3.5
1	D	163	SER	3.4
1	C	66	ASP	3.3
1	D	89	LEU	3.3
1	D	66	ASP	3.2
1	B	24	LYS	3.2
1	D	164	ARG	3.2
1	D	159	ALA	3.1
1	D	65	ASN	3.0
1	D	25	PRO	3.0
1	A	252	ARG	2.9
1	A	166	GLN	2.8
1	D	81	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	69	GLU	2.8
1	A	25	PRO	2.8
1	B	200	ARG	2.7
1	D	160	PHE	2.7
1	D	226	TYR	2.7
1	C	150	LYS	2.7
1	B	23	ASP	2.6
1	C	166	GLN	2.6
1	D	7	ILE	2.6
1	D	46	ILE	2.6
1	D	26	LEU	2.6
1	D	70	TRP	2.6
1	D	48	GLY	2.5
1	D	69	GLU	2.5
1	B	119	PRO	2.5
1	D	24	LYS	2.5
1	D	216	TYR	2.4
1	C	67	LYS	2.4
1	D	49	PHE	2.4
1	D	162	SER	2.4
1	A	68	GLY	2.3
1	A	164	ARG	2.3
1	D	27	TYR	2.2
1	D	108	LEU	2.2
1	A	5	THR	2.2
1	B	22	SER	2.2
1	B	252	ARG	2.2
1	D	47	LEU	2.1
1	D	90	THR	2.1
1	A	253	GLY	2.1
1	D	59	GLY	2.1
1	D	78	ILE	2.1
1	D	56	VAL	2.0
1	D	166	GLN	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	D	602	5/5	0.93	0.11	68,68,68,68	0
3	GLU	A	504	10/10	0.95	0.14	31,33,34,35	0
2	SO4	C	603	5/5	0.97	0.09	55,56,57,57	0
2	SO4	A	604	5/5	0.98	0.10	54,55,56,56	0
2	SO4	B	601[A]	5/5	0.98	0.09	27,27,28,28	5
3	GLU	A	501	10/10	0.98	0.09	12,16,18,19	0
3	GLU	A	502	10/10	0.98	0.10	11,13,15,16	0
2	SO4	B	601[B]	5/5	0.98	0.09	31,31,32,32	5
3	GLU	A	503	10/10	0.99	0.07	17,18,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.