



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 12:46 PM BST

PDB ID : 3UNW
Title : Crystal Structure of Human GAC in Complex with Glutamate
Authors : DeLaBarre, B.; Gross, S.; Cheng, F.; Gao, Y.; Jha, A.; Jiang, F.; Song, J.J.;
Wie, W.; Hurov, J.
Deposited on : 2011-11-16
Resolution : 2.56 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 : 2.14.4.dev1
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) : 2.14.4.dev1

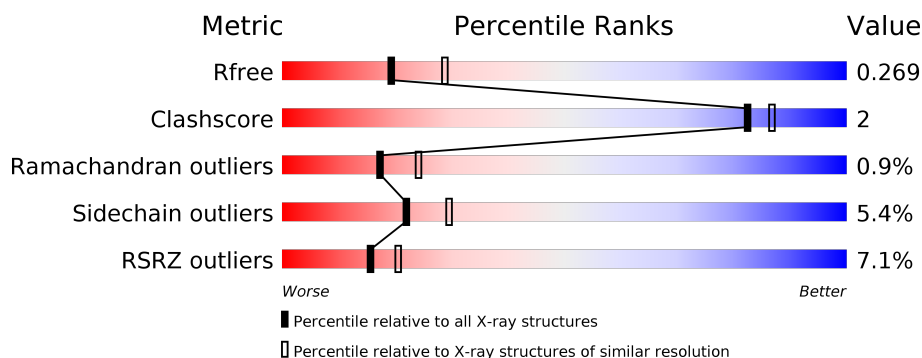
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	534	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>9%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	534	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>8%</div> <div>••</div> <div>25%</div> </div> </div>
1	C	534	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>10%</div> <div>•</div> <div>25%</div> </div> </div>
1	D	534	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>11%</div> <div>•</div> <div>25%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12769 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	9	0	0
			3162	2014	532	588	28			
1	B	400	Total	C	N	O	S	6	0	0
			3123	1993	525	577	28			
1	C	400	Total	C	N	O	S	25	0	0
			3124	1995	525	576	28			
1	D	403	Total	C	N	O	S	13	0	0
			3141	2001	528	584	28			

There are 24 discrepancies between the modelled and reference sequences:

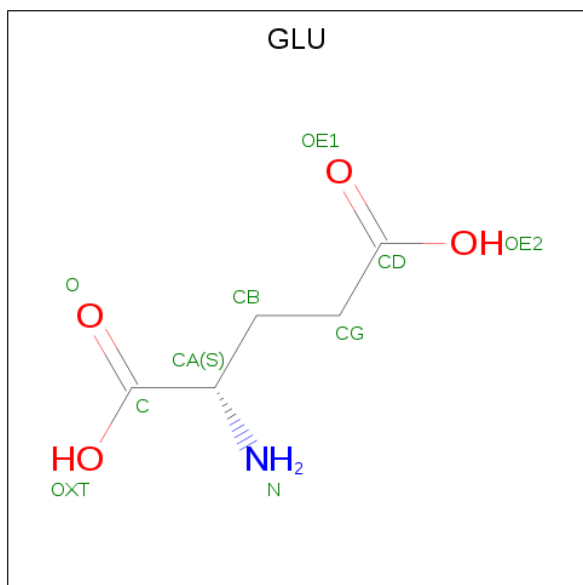
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	HIS	-	EXPRESSION TAG	UNP O94925
A	600	HIS	-	EXPRESSION TAG	UNP O94925
A	601	HIS	-	EXPRESSION TAG	UNP O94925
A	602	HIS	-	EXPRESSION TAG	UNP O94925
A	603	HIS	-	EXPRESSION TAG	UNP O94925
A	604	HIS	-	EXPRESSION TAG	UNP O94925
B	599	HIS	-	EXPRESSION TAG	UNP O94925
B	600	HIS	-	EXPRESSION TAG	UNP O94925
B	601	HIS	-	EXPRESSION TAG	UNP O94925
B	602	HIS	-	EXPRESSION TAG	UNP O94925
B	603	HIS	-	EXPRESSION TAG	UNP O94925
B	604	HIS	-	EXPRESSION TAG	UNP O94925
C	599	HIS	-	EXPRESSION TAG	UNP O94925
C	600	HIS	-	EXPRESSION TAG	UNP O94925
C	601	HIS	-	EXPRESSION TAG	UNP O94925
C	602	HIS	-	EXPRESSION TAG	UNP O94925
C	603	HIS	-	EXPRESSION TAG	UNP O94925
C	604	HIS	-	EXPRESSION TAG	UNP O94925
D	599	HIS	-	EXPRESSION TAG	UNP O94925
D	600	HIS	-	EXPRESSION TAG	UNP O94925
D	601	HIS	-	EXPRESSION TAG	UNP O94925

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	602	HIS	-	EXPRESSION TAG	UNP O94925
D	603	HIS	-	EXPRESSION TAG	UNP O94925
D	604	HIS	-	EXPRESSION TAG	UNP O94925

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



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

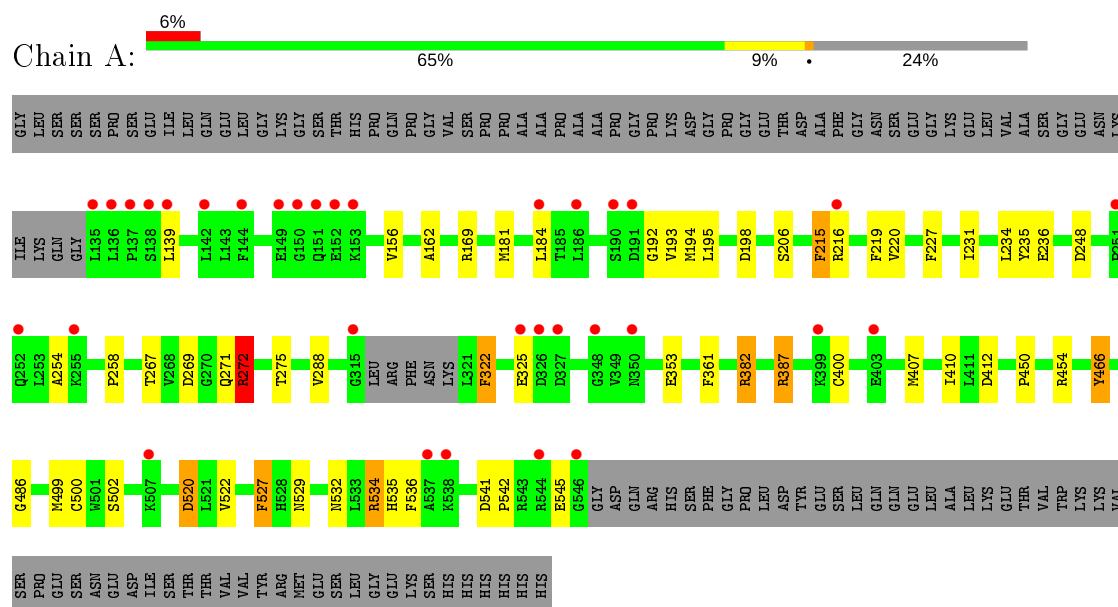
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	43	Total	O	0	0
			43	43		
3	C	46	Total	O	0	0
			46	46		
3	D	44	Total	O	0	0
			44	44		

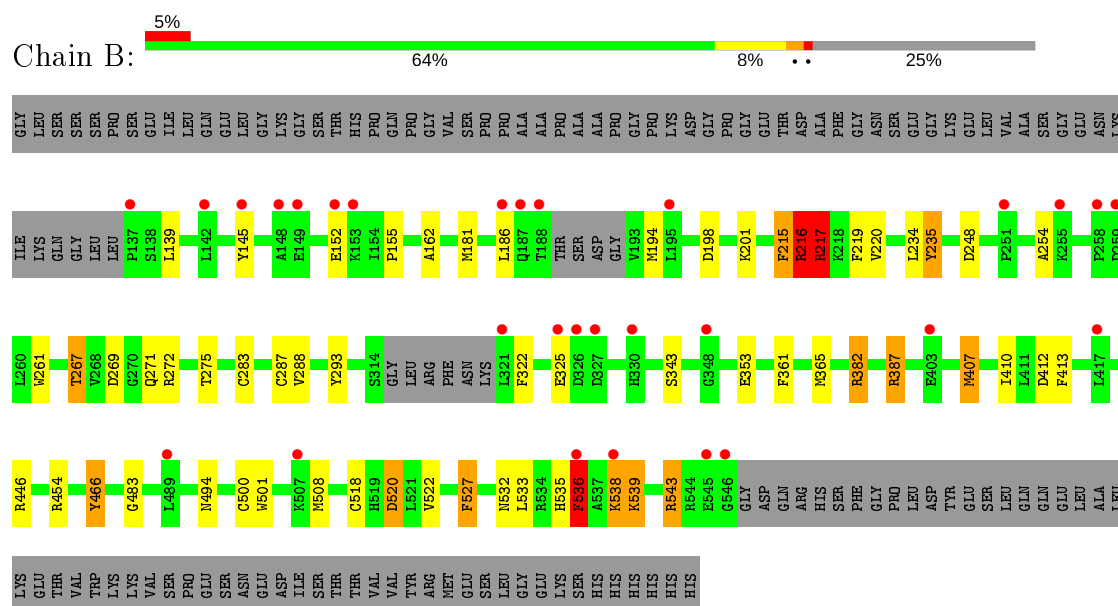
3 Residue-property plots [i](#)

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.

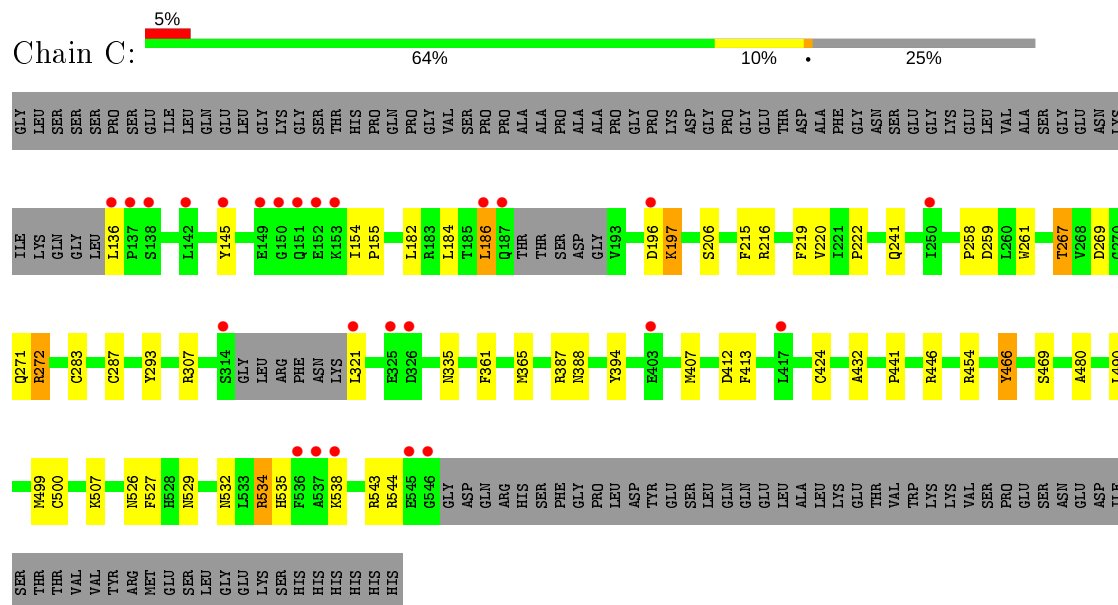
- Molecule 1: Glutaminase kidney isoform, mitochondrial



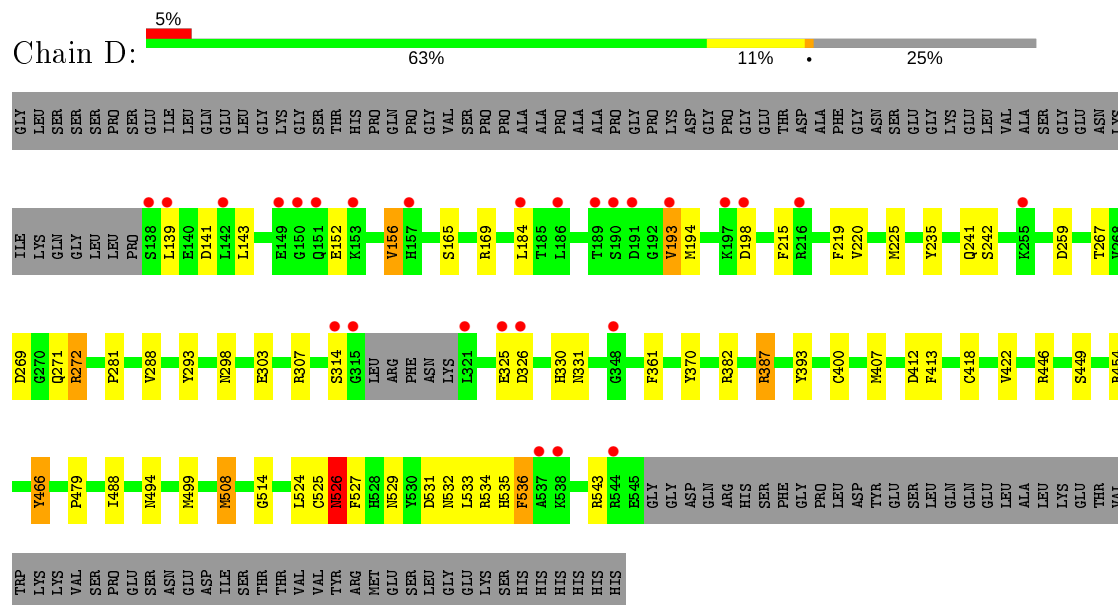
- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.66Å 139.61Å 178.38Å 90.00° 94.14° 90.00°	Depositor
Resolution (Å)	29.04 – 2.56 29.28 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.04-2.56) 99.6 (29.28-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.261 0.232 , 0.269	Depositor DCC
R_{free} test set	4004 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12769	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 5.76% 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

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	1.08	2/3232 (0.1%)	1.12	19/4364 (0.4%)
1	B	1.08	5/3192 (0.2%)	1.13	24/4307 (0.6%)
1	C	1.08	4/3193 (0.1%)	1.10	18/4309 (0.4%)
1	D	1.09	3/3210 (0.1%)	1.09	16/4333 (0.4%)
All	All	1.08	14/12827 (0.1%)	1.11	77/17313 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	10
1	C	0	5
1	D	0	12
All	All	0	34

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	500	CYS	CB-SG	-9.32	1.66	1.82
1	A	500	CYS	CB-SG	-7.51	1.69	1.82
1	C	283	CYS	CB-SG	-6.96	1.70	1.82
1	D	400	CYS	CB-SG	-6.92	1.70	1.82
1	D	525	CYS	CB-SG	-6.81	1.70	1.82
1	C	500	CYS	CB-SG	-6.77	1.70	1.82
1	C	424	CYS	CB-SG	-6.05	1.72	1.82
1	B	283	CYS	CB-SG	-5.84	1.72	1.81
1	A	400	CYS	CB-SG	-5.64	1.72	1.81
1	C	287	CYS	CB-SG	-5.49	1.72	1.81
1	B	518	CYS	CB-SG	-5.40	1.73	1.81
1	B	501	TRP	NE1-CE2	-5.24	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	483	GLY	N-CA	-5.07	1.38	1.46
1	D	479	PRO	N-CD	-5.02	1.40	1.47

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TYR	CB-CG-CD2	-10.14	114.91	121.00
1	A	466	TYR	CB-CG-CD2	-9.75	115.15	121.00
1	B	543	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	C	534	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	B	466	TYR	CB-CG-CD1	9.42	126.65	121.00
1	A	466	TYR	CB-CG-CD1	8.70	126.22	121.00
1	B	194	MET	CG-SD-CE	-8.60	86.44	100.20
1	A	194	MET	CG-SD-CE	-8.53	86.55	100.20
1	A	454	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	D	466	TYR	CB-CG-CD2	-8.14	116.12	121.00
1	C	543	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	194	MET	CG-SD-CE	-7.79	87.74	100.20
1	C	466	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	D	466	TYR	CB-CG-CD1	7.72	125.63	121.00
1	D	534	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	219	PHE	CB-CG-CD1	7.59	126.12	120.80
1	D	387	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	527	PHE	CB-CG-CD2	-7.37	115.64	120.80
1	D	215	PHE	CB-CG-CD2	7.37	125.96	120.80
1	B	387	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	407	MET	CG-SD-CE	-7.21	88.67	100.20
1	C	466	TYR	CB-CG-CD1	7.03	125.22	121.00
1	C	219	PHE	CB-CG-CD2	-7.00	115.90	120.80
1	A	534	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	527	PHE	CB-CG-CD2	-6.88	115.98	120.80
1	B	536	PHE	CB-CG-CD1	-6.87	115.99	120.80
1	D	508	MET	CG-SD-CE	-6.79	89.33	100.20
1	B	527	PHE	CB-CG-CD1	6.79	125.55	120.80
1	A	219	PHE	CB-CG-CD2	-6.73	116.09	120.80
1	A	215	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	C	413	PHE	CB-CG-CD2	-6.69	116.12	120.80
1	B	219	PHE	CB-CG-CD1	6.52	125.36	120.80
1	A	322	PHE	CB-CG-CD1	6.50	125.35	120.80
1	A	272	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	D	219	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	D	527	PHE	CB-CG-CD2	-6.26	116.42	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	543	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	536	PHE	CB-CG-CD2	6.17	125.12	120.80
1	C	446	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	215	PHE	CB-CG-CD1	-6.08	116.54	120.80
1	B	508	MET	CG-SD-CE	-6.04	90.54	100.20
1	A	387	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	527	PHE	CB-CG-CD1	5.94	124.96	120.80
1	C	454	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	522	VAL	CA-CB-CG2	-5.81	102.18	110.90
1	B	543	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	219	PHE	CB-CG-CD1	5.75	124.83	120.80
1	B	219	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	C	413	PHE	CB-CG-CD1	5.70	124.79	120.80
1	D	543	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	365	MET	CG-SD-CE	5.68	109.29	100.20
1	C	365	MET	CG-SD-CE	5.66	109.26	100.20
1	A	215	PHE	CB-CG-CD2	5.66	124.76	120.80
1	C	454	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	216	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	446	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	413	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	C	293	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	C	145	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	272	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	215	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	C	215	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	C	527	PHE	CB-CG-CD1	5.42	124.59	120.80
1	A	181	MET	CG-SD-CE	-5.34	91.66	100.20
1	D	219	PHE	CB-CG-CD1	5.33	124.53	120.80
1	D	526	ASN	CA-CB-CG	5.29	125.03	113.40
1	B	413	PHE	CB-CG-CD1	5.24	124.47	120.80
1	A	322	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	A	499	MET	CG-SD-CE	5.20	108.52	100.20
1	B	407	MET	CA-CB-CG	5.18	122.11	113.30
1	B	522	VAL	CA-CB-CG2	-5.16	103.17	110.90
1	C	261	TRP	CA-CB-CG	5.14	123.47	113.70
1	D	413	PHE	CB-CG-CD1	5.10	124.37	120.80
1	B	181	MET	CG-SD-CE	-5.07	92.09	100.20
1	B	215	PHE	CB-CG-CD2	5.06	124.34	120.80
1	D	393	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	C	272	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ARG	Sidechain
1	A	235	TYR	Sidechain
1	A	272	ARG	Sidechain
1	A	382	ARG	Sidechain
1	A	466	TYR	Sidechain
1	A	534	ARG	Sidechain
1	A	536	PHE	Mainchain
1	B	145	TYR	Sidechain
1	B	216	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	235	TYR	Sidechain
1	B	293	TYR	Sidechain
1	B	382	ARG	Sidechain
1	B	454	ARG	Sidechain
1	B	466	TYR	Sidechain
1	B	535	HIS	Mainchain
1	B	543	ARG	Sidechain
1	C	272	ARG	Sidechain
1	C	394	TYR	Sidechain
1	C	466	TYR	Sidechain
1	C	534	ARG	Sidechain
1	C	544	ARG	Sidechain
1	D	169	ARG	Sidechain
1	D	235	TYR	Sidechain
1	D	272	ARG	Sidechain
1	D	293	TYR	Sidechain
1	D	370	TYR	Sidechain
1	D	382	ARG	Sidechain
1	D	446	ARG	Sidechain
1	D	454	ARG	Sidechain
1	D	466	TYR	Sidechain
1	D	524	LEU	Mainchain
1	D	526	ASN	Mainchain
1	D	536	PHE	Mainchain

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	3162	0	3126	16	6
1	B	3123	0	3100	18	1
1	C	3124	0	3103	14	8
1	D	3141	0	3112	19	3
2	A	10	0	5	0	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	D	10	0	5	1	0
3	A	46	0	0	0	0
3	B	43	0	0	0	0
3	C	46	0	0	0	0
3	D	44	0	0	0	1
All	All	12769	0	12461	62	12

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 2.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASN:HD22	1:A:535:HIS:H	1.18	0.91
1:C:532:ASN:HD22	1:C:535:HIS:H	1.24	0.85
1:A:267:THR:HG22	1:A:269:ASP:H	1.43	0.81
1:D:267:THR:HG22	1:D:269:ASP:H	1.46	0.80
1:B:267:THR:HG22	1:B:269:ASP:H	1.50	0.77
1:B:267:THR:HG21	1:B:271:GLN:OE1	1.95	0.66
1:B:272:ARG:HH11	1:B:272:ARG:HG2	1.61	0.64
1:D:298:ASN:HD22	1:D:449:SER:H	1.50	0.60
1:C:267:THR:HG22	1:C:269:ASP:H	1.67	0.59
1:D:156:VAL:HB	1:D:193:VAL:HG22	1.84	0.59
1:A:529:ASN:HD21	1:C:529:ASN:HD21	1.50	0.59
1:B:216:ARG:HA	1:B:216:ARG:HH11	1.67	0.59
1:D:532:ASN:HD22	1:D:535:HIS:H	1.49	0.58
1:A:267:THR:HG22	1:A:269:ASP:N	2.20	0.53
1:B:494:ASN:ND2	1:D:533:LEU:H	2.07	0.53
1:B:267:THR:HG22	1:B:269:ASP:N	2.23	0.52
1:D:418:CYS:HG	2:D:800:GLU:N	2.09	0.50
1:A:267:THR:HG21	1:A:271:GLN:OE1	2.11	0.50
1:D:267:THR:HG22	1:D:269:ASP:N	2.22	0.49
1:C:267:THR:HG21	1:C:271:GLN:OE1	2.13	0.48
1:D:267:THR:CG2	1:D:269:ASP:H	2.21	0.48
1:B:267:THR:CG2	1:B:269:ASP:H	2.23	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:ASN:HD22	1:D:535:HIS:N	2.10	0.48
1:D:267:THR:HG21	1:D:271:GLN:OE1	2.13	0.48
1:C:532:ASN:ND2	1:C:535:HIS:H	2.03	0.47
1:B:533:LEU:H	1:D:494:ASN:ND2	2.12	0.47
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.79	0.47
1:B:220:VAL:CG1	1:B:267:THR:HG23	2.45	0.47
1:D:526:ASN:HA	1:D:531:ASP:OD2	2.14	0.47
1:D:165:SER:HB2	1:D:225:MET:SD	2.55	0.47
1:D:281:PRO:HA	1:D:422:VAL:O	2.16	0.46
1:A:220:VAL:CG1	1:A:267:THR:HG23	2.46	0.46
1:C:197:LYS:HD2	1:C:197:LYS:C	2.36	0.46
1:C:220:VAL:CG1	1:C:267:THR:HG23	2.46	0.46
1:C:267:THR:HG22	1:C:269:ASP:N	2.29	0.45
1:C:154:ILE:HG22	1:C:155:PRO:O	2.16	0.45
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.99	0.45
1:D:220:VAL:CG1	1:D:267:THR:HG23	2.47	0.44
1:A:529:ASN:HD21	1:C:529:ASN:ND2	2.14	0.44
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.99	0.44
1:A:410:ILE:HD13	1:A:410:ILE:HA	1.90	0.43
1:C:480:ALA:HB2	1:C:490:LEU:HD12	2.00	0.43
1:B:216:ARG:O	1:B:217:ARG:HB2	2.18	0.43
1:B:343:SER:HA	1:B:410:ILE:HD12	2.00	0.43
1:B:536:PHE:CD2	1:B:536:PHE:N	2.83	0.43
1:B:538:LYS:O	1:B:539:LYS:HG3	2.18	0.43
1:A:227:PHE:CZ	1:A:231:ILE:HD11	2.54	0.42
1:C:432:ALA:HB1	1:C:441:PRO:HG3	2.01	0.42
1:B:235:TYR:CE1	1:B:261:TRP:CD1	3.07	0.42
1:A:486:GLY:HA3	1:A:502:SER:O	2.20	0.42
1:B:248:ASP:HA	1:B:254:ALA:HB2	2.00	0.42
1:C:182:LEU:O	1:C:186:LEU:HB2	2.19	0.42
1:A:248:ASP:HA	1:A:254:ALA:HB2	2.02	0.42
1:A:272:ARG:HH11	1:A:272:ARG:HG2	1.85	0.41
1:C:335:ASN:HD22	1:C:388:ASN:HD21	1.68	0.41
1:B:532:ASN:HA	1:D:494:ASN:HD21	1.85	0.41
1:D:314:SER:HB3	1:D:330:HIS:CG	2.56	0.41
1:D:330:HIS:O	1:D:331:ASN:HB3	2.21	0.40
1:D:488:ILE:HD12	1:D:514:GLY:HA3	2.03	0.40
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.87	0.40
1:A:541:ASP:HA	1:A:542:PRO:HD2	1.84	0.40
1:A:527:PHE:CZ	1:A:542:PRO:HG2	2.56	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:CD	1:C:538:LYS:NZ[1_455]	0.60	1.60
1:A:236:GLU:OE1	1:C:538:LYS:NZ[1_455]	0.69	1.51
1:C:259:ASP:OD1	1:C:307:ARG:NH2[1_655]	1.32	0.88
1:D:259:ASP:OD1	1:D:307:ARG:NH2[1_455]	1.44	0.76
1:A:236:GLU:OE1	1:C:538:LYS:CE[1_455]	1.54	0.66
1:A:236:GLU:OE2	1:C:538:LYS:NZ[1_455]	1.55	0.65
1:A:236:GLU:CD	1:C:538:LYS:CE[1_455]	1.92	0.28
1:A:236:GLU:CG	1:C:538:LYS:NZ[1_455]	1.98	0.22
1:D:259:ASP:CG	1:D:307:ARG:NH2[1_455]	2.07	0.13
1:C:259:ASP:CG	1:C:307:ARG:NH2[1_655]	2.12	0.08
1:D:242:SER:CB	1:D:303:GLU:OE2[1_455]	2.17	0.03
1:B:198:ASP:OD2	3:D:70:HOH:O[2_556]	2.18	0.02

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	403/534 (76%)	384 (95%)	17 (4%)	2 (0%)	29	39
1	B	394/534 (74%)	373 (95%)	16 (4%)	5 (1%)	12	15
1	C	394/534 (74%)	374 (95%)	15 (4%)	5 (1%)	12	15
1	D	399/534 (75%)	383 (96%)	14 (4%)	2 (0%)	29	39
All	All	1590/2136 (74%)	1514 (95%)	62 (4%)	14 (1%)	17	24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	VAL
1	B	217	ARG
1	B	322	PHE
1	B	527	PHE
1	D	193	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	192	GLY
1	C	241	GLN
1	C	469	SER
1	B	539	LYS
1	B	287	CYS
1	C	222	PRO
1	C	186	LEU
1	D	241	GLN
1	C	526	ASN

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	350/458 (76%)	328 (94%)	22 (6%)	18	23
1	B	347/458 (76%)	328 (94%)	19 (6%)	21	29
1	C	347/458 (76%)	332 (96%)	15 (4%)	29	39
1	D	349/458 (76%)	329 (94%)	20 (6%)	20	27
All	All	1393/1832 (76%)	1317 (94%)	76 (6%)	22	29

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LEU
1	A	156	VAL
1	A	184	LEU
1	A	195	LEU
1	A	198	ASP
1	A	206	SER
1	A	216	ARG
1	A	258	PRO
1	A	272	ARG
1	A	275	THR
1	A	288	VAL
1	A	322	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	325	GLU
1	A	353	GLU
1	A	361	PHE
1	A	382	ARG
1	A	387	ARG
1	A	407	MET
1	A	412	ASP
1	A	450	PRO
1	A	520	ASP
1	A	545	GLU
1	B	139	LEU
1	B	152	GLU
1	B	155	PRO
1	B	186	LEU
1	B	201	LYS
1	B	216	ARG
1	B	267	THR
1	B	275	THR
1	B	288	VAL
1	B	325	GLU
1	B	353	GLU
1	B	361	PHE
1	B	382	ARG
1	B	387	ARG
1	B	407	MET
1	B	412	ASP
1	B	520	ASP
1	B	536	PHE
1	B	538	LYS
1	C	136	LEU
1	C	184	LEU
1	C	196	ASP
1	C	197	LYS
1	C	206	SER
1	C	216	ARG
1	C	258	PRO
1	C	267	THR
1	C	321	LEU
1	C	361	PHE
1	C	387	ARG
1	C	407	MET
1	C	412	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	499	MET
1	C	507	LYS
1	D	139	LEU
1	D	141	ASP
1	D	143	LEU
1	D	152	GLU
1	D	156	VAL
1	D	184	LEU
1	D	198	ASP
1	D	272	ARG
1	D	288	VAL
1	D	325	GLU
1	D	326	ASP
1	D	361	PHE
1	D	387	ARG
1	D	407	MET
1	D	412	ASP
1	D	499	MET
1	D	508	MET
1	D	526	ASN
1	D	529	ASN
1	D	536	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	GLN
1	A	510	ASN
1	A	529	ASN
1	A	532	ASN
1	B	471	GLN
1	B	494	ASN
1	B	510	ASN
1	B	529	ASN
1	C	335	ASN
1	C	388	ASN
1	C	471	GLN
1	C	510	ASN
1	C	529	ASN
1	C	532	ASN
1	D	157	HIS
1	D	298	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	494	ASN
1	D	510	ASN
1	D	526	ASN
1	D	532	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	GLU	D	800	-	2,9,9	0.33	0	2,11,11	0.92	0
2	GLU	B	800	-	2,9,9	0.65	0	2,11,11	1.72	0
2	GLU	C	800	-	2,9,9	0.09	0	2,11,11	0.87	0
2	GLU	A	800	-	2,9,9	0.99	0	2,11,11	0.52	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
2	GLU	D	800	-	-	1/3/9/9	-
2	GLU	B	800	-	-	0/3/9/9	-
2	GLU	C	800	-	-	0/3/9/9	-
2	GLU	A	800	-	-	1/3/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	GLU	CA-CB-CG-CD
2	D	800	GLU	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	800	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	407/534 (76%)	0.40	33 (8%) 12 16	24, 39, 81, 96	2 (0%)
1	B	400/534 (74%)	0.37	29 (7%) 15 19	24, 39, 78, 89	1 (0%)
1	C	400/534 (74%)	0.32	25 (6%) 20 25	24, 39, 78, 92	6 (1%)
1	D	403/534 (75%)	0.28	27 (6%) 17 22	24, 39, 78, 89	3 (0%)
All	All	1610/2136 (75%)	0.34	114 (7%) 16 20	24, 39, 79, 96	12 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ASP	8.0
1	C	546	GLY	6.6
1	A	136	LEU	6.3
1	A	137	PRO	6.2
1	B	152	GLU	6.1
1	C	321	LEU	5.6
1	A	190	SER	5.6
1	A	135	LEU	5.6
1	A	150	GLY	5.4
1	C	152	GLU	5.4
1	B	325	GLU	5.4
1	D	138	SER	5.3
1	B	186	LEU	5.2
1	B	137	PRO	5.1
1	D	315	GLY	5.0
1	B	326	ASP	4.9
1	B	188	THR	4.9
1	C	537	ALA	4.9
1	D	190	SER	4.9
1	A	138	SER	4.8
1	B	149	GLU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	325	GLU	4.6
1	C	137	PRO	4.6
1	C	326	ASP	4.5
1	C	145	TYR	4.5
1	D	191	ASP	4.3
1	C	186	LEU	4.2
1	B	538	LYS	4.2
1	B	187	GLN	4.2
1	B	153	LYS	4.1
1	A	152	GLU	4.1
1	D	325	GLU	4.1
1	C	314	SER	4.0
1	C	325	GLU	3.9
1	B	142	LEU	3.8
1	A	255	LYS	3.8
1	B	195	LEU	3.8
1	A	538	LYS	3.7
1	B	546	GLY	3.6
1	B	348	GLY	3.6
1	D	151	GLN	3.6
1	D	321	LEU	3.5
1	C	187	GLN	3.5
1	D	142	LEU	3.3
1	C	545	GLU	3.3
1	B	403	GLU	3.3
1	C	538	LYS	3.2
1	A	327	ASP	3.2
1	A	537	ALA	3.2
1	B	145	TYR	3.1
1	B	321	LEU	3.1
1	C	153	LYS	3.1
1	B	545	GLU	3.0
1	A	546	GLY	3.0
1	D	326	ASP	3.0
1	C	136	LEU	3.0
1	A	315	GLY	3.0
1	A	399	LYS	3.0
1	B	251	PRO	3.0
1	D	255	LYS	3.0
1	C	151	GLN	3.0
1	A	326	ASP	2.9
1	A	186	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	150	GLY	2.8
1	B	417	LEU	2.8
1	A	149	GLU	2.8
1	A	139	LEU	2.8
1	D	157	HIS	2.7
1	D	149	GLU	2.7
1	C	196	ASP	2.7
1	C	142	LEU	2.7
1	A	216	ARG	2.6
1	C	138	SER	2.6
1	A	251	PRO	2.6
1	A	350	ASN	2.6
1	A	144	PHE	2.6
1	B	259	ASP	2.6
1	D	150	GLY	2.6
1	A	507	LYS	2.5
1	B	507	LYS	2.5
1	B	148	ALA	2.5
1	D	537	ALA	2.5
1	D	544	ARG	2.5
1	D	193	VAL	2.5
1	D	314	SER	2.5
1	A	153	LYS	2.5
1	D	538	LYS	2.5
1	D	153	LYS	2.4
1	C	536	PHE	2.4
1	D	348	GLY	2.4
1	A	403	GLU	2.4
1	B	489	LEU	2.4
1	B	330	HIS	2.3
1	B	327	ASP	2.3
1	D	198	ASP	2.3
1	A	151	GLN	2.3
1	D	184	LEU	2.3
1	A	544	ARG	2.3
1	A	184	LEU	2.3
1	C	417	LEU	2.3
1	C	149	GLU	2.2
1	D	189	THR	2.2
1	D	139	LEU	2.2
1	D	216	ARG	2.2
1	A	348	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	536	PHE	2.1
1	D	197	LYS	2.1
1	A	252	GLN	2.1
1	A	142	LEU	2.1
1	B	258	PRO	2.1
1	C	403	GLU	2.1
1	C	250	ILE	2.0
1	D	186	LEU	2.0
1	B	255	LYS	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 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(\AA^2)	Q<0.9
2	GLU	D	800	10/10	0.77	0.30	61,69,70,71	0
2	GLU	C	800	10/10	0.79	0.28	48,64,66,66	0
2	GLU	B	800	10/10	0.85	0.28	49,60,61,61	0
2	GLU	A	800	10/10	0.85	0.22	60,63,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.