



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:27 PM UTC

PDB ID : 3IHB / pdb_00003ihb
Title : Crystal Structure Analysis of Mglu in its tris and glutamate form
Authors : Yoshimune, K.; Shirakihara, Y.
Deposited on : 2009-07-29
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

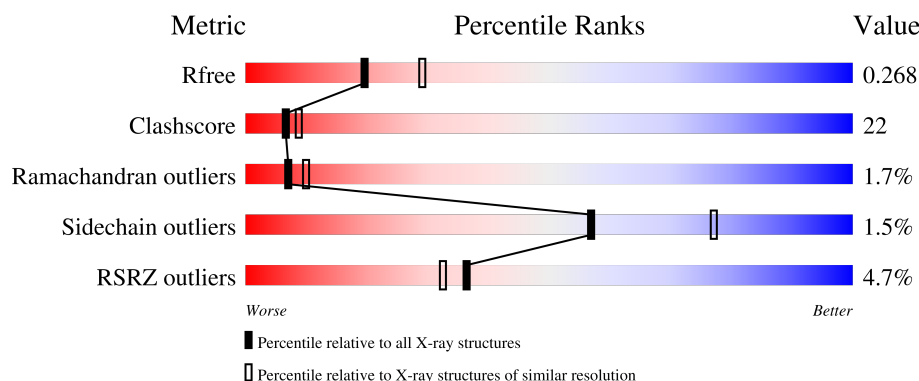
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	456	5% 66% 30% ..
1	B	456	4% 61% 34% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	B	500	-	-	X	-
3	TRS	A	600	-	X	-	-
3	TRS	B	600	-	X	-	-

2 Entry composition [i](#)

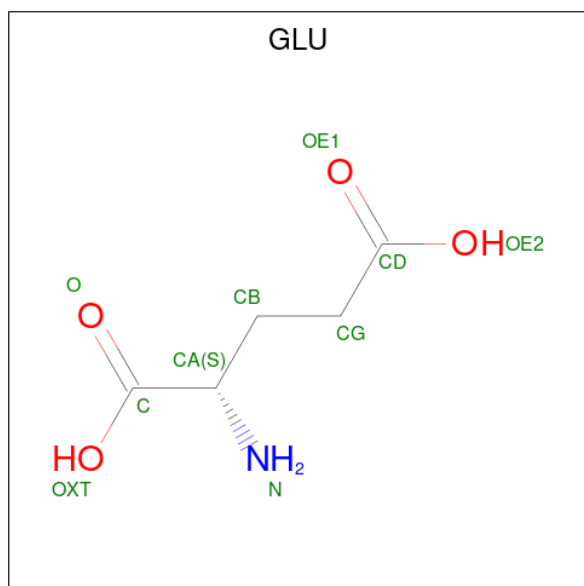
There are 4 unique types of molecules in this entry. The entry contains 7222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Salt-tolerant glutaminase.

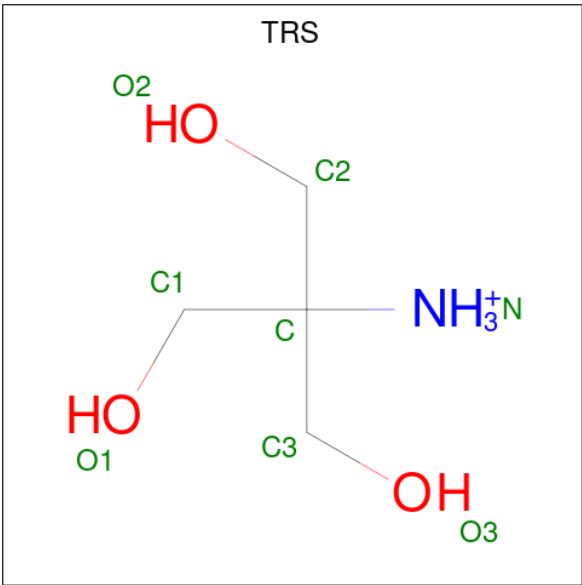
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3346	2078	613	640	15			
1	B	448	Total	C	N	O	S	0	0	0
			3331	2067	611	638	15			

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	1	3		
2	B	1	Total	C	N	O	0	0
			9	5	1	3		

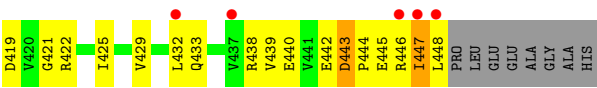
- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	267	Total	O	0	0
			267	267		
4	B	244	Total	O	0	0
			244	244		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.36Å 141.20Å 76.11Å 90.00° 105.37° 90.00°	Depositor
Resolution (Å)	19.86 – 2.40 19.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.86-2.40) 99.3 (19.86-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.30Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.221 , 0.268 0.221 , 0.268	Depositor DCC
R_{free} test set	2641 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7222	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.59% 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: TRS

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	0.43	0/3400	0.99	21/4617 (0.5%)
1	B	0.44	0/3384	1.00	19/4594 (0.4%)
All	All	0.44	0/6784	0.99	40/9211 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	LEU	N-CA-C	8.93	129.82	110.80
1	B	109	ASP	N-CA-C	7.68	119.29	111.07
1	A	109	ASP	N-CA-C	7.60	120.23	111.11
1	B	273	VAL	N-CA-C	7.04	117.75	107.75
1	A	124	LEU	N-CA-C	7.00	125.71	110.80
1	A	124	LEU	CA-C-N	-6.79	115.97	123.16
1	A	124	LEU	C-N-CA	-6.79	115.97	123.16
1	A	325	ASP	N-CA-C	-6.78	105.14	113.41
1	A	137	ARG	N-CA-C	-6.09	104.75	111.82
1	B	316	ALA	N-CA-C	-5.93	105.30	112.54
1	A	309	GLY	N-CA-C	5.87	118.23	111.36
1	B	325	ASP	N-CA-C	-5.80	106.75	113.88
1	B	137	ARG	N-CA-C	-5.74	104.63	111.69
1	B	279	SER	CA-C-N	5.66	126.92	119.84
1	B	279	SER	C-N-CA	5.66	126.92	119.84
1	A	217	HIS	CA-C-N	5.66	125.33	119.56
1	A	217	HIS	C-N-CA	5.66	125.33	119.56
1	A	316	ALA	N-CA-C	-5.64	105.28	111.82
1	B	96	PHE	N-CA-C	5.59	118.74	109.46
1	A	360	GLY	N-CA-C	-5.58	107.00	114.25
1	A	35	ASP	CA-C-N	5.57	125.19	119.56
1	A	35	ASP	C-N-CA	5.57	125.19	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	LYS	CA-C-N	-5.46	114.13	119.64
1	B	67	LYS	C-N-CA	-5.46	114.13	119.64
1	B	80	PHE	N-CA-C	5.41	116.86	111.07
1	B	107	ARG	N-CA-C	5.32	114.97	108.11
1	B	335	ILE	N-CA-C	5.29	116.37	108.54
1	B	443	ASP	CA-C-N	5.22	125.53	119.47
1	B	443	ASP	C-N-CA	5.22	125.53	119.47
1	A	71	TYR	N-CA-C	-5.21	105.68	111.36
1	A	243	TYR	CB-CA-C	-5.19	110.61	116.63
1	B	445	GLU	N-CA-C	5.15	116.33	108.30
1	A	193	ALA	N-CA-C	-5.13	105.77	111.36
1	A	279	SER	CA-C-N	5.13	126.25	119.84
1	A	279	SER	C-N-CA	5.13	126.25	119.84
1	B	272	ARG	N-CA-C	5.11	121.69	110.80
1	A	335	ILE	N-CA-C	5.07	115.98	108.23
1	A	63	GLN	CB-CA-C	-5.05	110.73	116.54
1	A	203	ASP	N-CA-C	-5.02	105.70	111.07
1	B	257	ALA	N-CA-C	5.00	116.68	109.07

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	3346	0	3330	131	0
1	B	3331	0	3312	156	1
2	A	9	0	5	3	0
2	B	9	0	5	7	0
3	A	8	0	11	2	0
3	B	8	0	11	5	0
4	A	267	0	0	18	0
4	B	244	0	0	24	0
All	All	7222	0	6674	289	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 22.

All (289) 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:62:ILE:HG21	1:A:142:MET:HE1	1.36	1.02
1:B:62:ILE:HG21	1:B:142:MET:HE1	1.50	0.93
1:B:112:MET:HE3	1:B:258:LYS:HD3	1.51	0.93
1:A:112:MET:HE3	1:A:258:LYS:HD3	1.51	0.92
1:B:356:LYS:HD2	1:B:356:LYS:O	1.68	0.91
1:A:222:GLU:HG3	1:A:224:MET:HE3	1.51	0.91
1:B:376:ARG:HG2	1:B:389:HIS:HB2	1.58	0.84
1:A:110:ASN:HD22	1:A:112:MET:H	1.26	0.84
1:A:201:VAL:HG23	4:A:582:HOH:O	1.77	0.83
1:B:411:LEU:HD11	1:B:448:LEU:HD12	1.61	0.80
1:A:86:GLN:HE21	1:A:179:VAL:HG13	1.48	0.78
1:B:201:VAL:HG23	4:B:530:HOH:O	1.83	0.78
1:B:110:ASN:HD22	1:B:112:MET:H	1.29	0.77
1:B:405:ARG:HD3	4:B:463:HOH:O	1.83	0.76
1:B:29:PRO:HG2	4:B:566:HOH:O	1.84	0.76
1:A:450:LEU:O	1:A:450:LEU:HD22	1.84	0.76
1:B:27:TYR:O	1:B:28:ILE:HG13	1.85	0.74
1:A:322:ARG:HD2	1:A:327:VAL:HG22	1.70	0.74
1:A:445:GLU:O	1:A:447:ILE:HG13	1.88	0.73
1:A:429:VAL:HG13	1:A:439:VAL:HG11	1.70	0.72
1:A:224:MET:HA	1:A:224:MET:HE2	1.73	0.71
1:B:110:ASN:ND2	1:B:112:MET:H	1.89	0.70
1:A:62:ILE:HD13	1:A:142:MET:HE3	1.73	0.70
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.57	0.70
1:B:222:GLU:OE2	1:B:224:MET:HE1	1.91	0.70
1:B:77:ASP:OD2	1:B:124:LEU:O	2.12	0.67
1:A:62:ILE:HD13	1:A:142:MET:CE	2.24	0.67
1:B:125:VAL:HB	1:B:129:ALA:HB2	1.76	0.67
1:A:401:ASP:HA	4:A:739:HOH:O	1.94	0.67
1:B:125:VAL:N	4:B:671:HOH:O	1.69	0.67
1:B:447:ILE:O	1:B:448:LEU:HB2	1.95	0.66
1:A:450:LEU:HD13	1:A:450:LEU:H	1.59	0.66
1:B:136:ASP:HB3	4:B:588:HOH:O	1.96	0.66
1:A:188:VAL:O	1:A:192:VAL:HG23	1.96	0.66
1:A:448:LEU:HB3	1:A:449:PRO:HD3	1.75	0.66
1:B:443:ASP:OD1	1:B:447:ILE:HG23	1.97	0.65
1:B:27:TYR:C	1:B:28:ILE:HG13	2.21	0.65
1:B:125:VAL:HB	1:B:129:ALA:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ARG:HD2	1:A:355:GLU:HB3	1.78	0.65
1:A:356:LYS:O	1:A:356:LYS:HD3	1.97	0.64
1:B:350:LEU:O	1:B:352:THR:N	2.29	0.64
1:A:361:TRP:CZ3	1:A:363:ALA:HA	2.33	0.64
1:B:105:SER:HB2	4:B:526:HOH:O	1.98	0.63
1:B:62:ILE:HD13	1:B:142:MET:HE3	1.81	0.63
1:A:28:ILE:HG22	1:A:30:VAL:HG12	1.80	0.62
1:A:277:VAL:HG11	1:A:291:GLY:HA2	1.81	0.62
1:A:103:ALA:HB3	4:A:533:HOH:O	1.99	0.62
1:B:63:GLN:HB3	2:B:500:GLU:HG3	1.81	0.62
1:A:297:ARG:NH2	4:A:717:HOH:O	2.20	0.61
1:A:395:ALA:HA	1:A:399:GLU:CG	2.29	0.61
1:B:64:SER:HB2	2:B:500:GLU:OE2	2.00	0.61
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.64	0.61
1:B:201:VAL:HG22	1:B:278:PHE:HB2	1.82	0.61
1:B:411:LEU:CD1	1:B:448:LEU:HD12	2.31	0.60
1:B:422:ARG:HD3	4:B:635:HOH:O	2.01	0.60
1:A:85:ARG:NH2	4:A:480:HOH:O	2.33	0.60
1:B:130:SER:OG	1:B:133:GLU:HG3	2.01	0.60
1:A:112:MET:HE3	1:A:258:LYS:CD	2.29	0.59
1:B:226:PRO:HA	3:B:600:TRS:H11	1.84	0.59
1:B:188:VAL:O	1:B:192:VAL:HG23	2.02	0.59
1:A:201:VAL:HG22	1:A:278:PHE:HB2	1.85	0.59
1:A:296:ARG:O	1:A:300:GLU:HG3	2.03	0.59
1:A:317:VAL:HG21	1:A:388:VAL:HG22	1.85	0.58
1:A:450:LEU:H	1:A:450:LEU:CD1	2.16	0.58
1:B:320:VAL:HB	1:B:390:GLU:HB3	1.85	0.58
1:B:329:LEU:HD23	1:B:409:LEU:CD2	2.32	0.58
1:A:110:ASN:ND2	1:A:112:MET:H	1.98	0.58
1:A:322:ARG:CD	1:A:327:VAL:HG22	2.33	0.57
1:B:223:ARG:HD3	3:B:600:TRS:H12	1.86	0.57
1:B:417:ILE:HD11	1:B:421:GLY:C	2.28	0.57
1:A:209:ALA:O	1:A:213:THR:HG23	2.04	0.57
1:B:433:GLN:HB3	4:B:655:HOH:O	2.05	0.57
1:B:425:ILE:O	1:B:429:VAL:HG23	2.04	0.57
1:B:339:GLY:O	1:B:343:VAL:HG23	2.05	0.57
1:B:226:PRO:HA	3:B:600:TRS:C1	2.35	0.57
1:B:261:VAL:HG22	2:B:500:GLU:HG2	1.87	0.57
1:B:320:VAL:HG22	1:B:329:LEU:CD1	2.35	0.57
1:A:85:ARG:HH11	1:A:85:ARG:HG2	1.70	0.56
1:A:322:ARG:HG2	1:A:322:ARG:HH21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:O	1:A:371:GLU:HG3	2.06	0.56
1:B:310:ASP:C	4:B:572:HOH:O	2.47	0.56
1:A:86:GLN:NE2	1:A:179:VAL:HG13	2.19	0.56
1:B:261:VAL:CG2	2:B:500:GLU:HG2	2.35	0.56
1:B:302:PHE:O	1:B:303:ARG:HB2	2.05	0.56
1:B:103:ALA:C	1:B:105:SER:H	2.14	0.56
1:A:220:THR:OG1	1:A:222:GLU:HG2	2.06	0.56
1:B:3:HIS:CE1	1:B:5:ILE:HG12	2.40	0.56
1:B:1:MET:N	4:B:494:HOH:O	2.34	0.56
1:A:320:VAL:HG22	1:A:329:LEU:HD13	1.88	0.55
1:A:363:ALA:HB1	1:A:370:GLN:OE1	2.06	0.55
1:A:12:LEU:HD11	1:A:297:ARG:HG3	1.88	0.55
1:A:445:GLU:HA	4:A:601:HOH:O	2.06	0.55
1:B:376:ARG:CG	1:B:389:HIS:HB2	2.31	0.55
1:B:237:MET:HE1	1:B:266:LEU:HD13	1.87	0.55
1:B:440:GLU:HG2	4:B:642:HOH:O	2.06	0.55
1:B:72:ALA:O	1:B:76:VAL:HG23	2.07	0.54
1:B:317:VAL:HG21	1:B:388:VAL:HG22	1.90	0.54
1:A:261:VAL:HG13	2:A:500:GLU:CD	2.33	0.54
1:B:429:VAL:HG13	1:B:439:VAL:HG11	1.88	0.54
1:B:352:THR:HG21	1:B:432:LEU:HD11	1.89	0.54
1:A:397:ARG:HH21	1:A:398:ASP:HA	1.73	0.54
1:B:315:THR:O	1:B:315:THR:HG22	2.08	0.54
1:B:368:ARG:NH2	1:B:371:GLU:OE2	2.40	0.53
1:B:106:HIS:HD2	4:B:605:HOH:O	1.92	0.53
1:B:353:GLY:HA3	1:B:355:GLU:OE2	2.08	0.53
1:A:226:PRO:HG2	1:A:229:VAL:CG2	2.39	0.53
1:A:153:ASP:HB2	1:A:198:LEU:HD11	1.91	0.53
1:B:78:ARG:HH11	1:B:78:ARG:HB3	1.74	0.53
1:B:261:VAL:HG13	2:B:500:GLU:CD	2.34	0.53
1:B:417:ILE:CG2	1:B:447:ILE:HG13	2.40	0.53
1:A:395:ALA:HA	1:A:399:GLU:HG2	1.89	0.52
1:B:446:ARG:O	1:B:447:ILE:C	2.52	0.52
1:B:103:ALA:C	1:B:105:SER:N	2.67	0.52
1:B:237:MET:CE	1:B:266:LEU:HD13	2.38	0.52
1:A:393:ALA:O	1:A:396:ALA:HB3	2.10	0.52
1:B:273:VAL:HG22	1:B:274:GLY:N	2.25	0.51
1:B:226:PRO:HG2	1:B:229:VAL:CG2	2.40	0.51
1:A:417:ILE:HD11	1:A:421:GLY:C	2.35	0.51
1:B:408:VAL:HG11	1:B:442:GLU:OE2	2.11	0.51
1:A:315:THR:HG22	1:A:315:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:MET:HE1	1:B:287:ASN:ND2	2.25	0.51
1:B:279:SER:OG	1:B:290:ARG:HD3	2.10	0.51
1:A:101:LEU:O	1:A:106:HIS:HA	2.11	0.51
1:A:357:PRO:HD2	4:A:637:HOH:O	2.11	0.51
1:B:28:ILE:HG22	1:B:30:VAL:HG12	1.92	0.51
1:B:30:VAL:N	4:B:566:HOH:O	2.41	0.50
1:B:417:ILE:HG22	1:B:447:ILE:HG13	1.93	0.50
1:B:310:ASP:CG	4:B:572:HOH:O	2.54	0.50
1:B:154:TRP:HA	1:B:157:TYR:HB3	1.93	0.50
1:B:329:LEU:HD23	1:B:409:LEU:HD21	1.92	0.50
1:A:422:ARG:HD3	1:A:449:PRO:O	2.11	0.50
1:B:320:VAL:HG11	1:B:391:ALA:HA	1.93	0.50
1:B:110:ASN:O	1:B:116:GLY:HA3	2.11	0.50
1:B:419:ASP:HA	1:B:422:ARG:HH11	1.76	0.50
1:A:166:ARG:O	1:A:169:SER:HB3	2.11	0.49
1:B:41:ILE:HA	1:B:201:VAL:HG11	1.93	0.49
1:B:333:GLY:O	1:B:414:VAL:HG13	2.11	0.49
1:B:284:GLU:H	1:B:284:GLU:CD	2.20	0.49
1:B:396:ALA:C	1:B:398:ASP:H	2.19	0.49
1:A:284:GLU:CD	1:A:284:GLU:H	2.20	0.49
1:A:358:GLY:O	1:A:359:THR:C	2.55	0.49
1:A:397:ARG:HE	1:A:397:ARG:C	2.20	0.49
1:A:440:GLU:HA	4:A:747:HOH:O	2.13	0.49
1:A:64:SER:HB2	2:A:500:GLU:OE2	2.12	0.49
1:B:46:PRO:HD2	4:B:607:HOH:O	2.12	0.49
1:A:77:ASP:OD2	1:A:124:LEU:O	2.31	0.49
1:A:394:ALA:O	1:A:398:ASP:HB2	2.13	0.49
1:B:201:VAL:HG13	1:B:276:GLY:C	2.37	0.49
1:A:429:VAL:HA	1:A:432:LEU:HD12	1.95	0.48
1:A:351:ARG:NH1	4:A:732:HOH:O	2.34	0.48
1:B:3:HIS:HE1	1:B:5:ILE:HG12	1.76	0.48
1:B:371:GLU:O	1:B:374:ALA:HB3	2.14	0.48
1:A:85:ARG:NH1	1:A:86:GLN:OE1	2.46	0.48
1:B:216:ILE:HD13	1:B:416:ARG:NH1	2.28	0.48
1:B:362:ASP:OD1	1:B:364:ALA:N	2.43	0.48
1:A:103:ALA:C	1:A:105:SER:H	2.22	0.48
1:B:29:PRO:HA	1:B:32:ALA:HB3	1.96	0.47
1:B:223:ARG:C	1:B:224:MET:HE2	2.39	0.47
1:A:191:TYR:O	1:A:194:GLN:HB3	2.14	0.47
1:B:296:ARG:O	1:B:300:GLU:HG3	2.14	0.47
1:B:312:LEU:HD12	1:B:315:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	1:A:182:ASP:OD1	2.45	0.47
1:A:69:PHE:CE1	1:A:207:MET:HE2	2.49	0.47
1:A:201:VAL:HG13	1:A:276:GLY:C	2.40	0.47
1:B:438:ARG:HG3	1:B:438:ARG:HH11	1.78	0.47
1:A:224:MET:HE2	1:A:224:MET:CA	2.44	0.47
1:B:201:VAL:CG1	1:B:276:GLY:O	2.63	0.47
1:B:63:GLN:OE1	2:B:500:GLU:N	2.48	0.47
1:B:331:LEU:HD12	1:B:411:LEU:CD2	2.45	0.47
1:B:393:ALA:O	1:B:396:ALA:HB3	2.16	0.46
1:A:335:ILE:O	1:A:417:ILE:HG13	2.15	0.46
1:B:191:TYR:O	1:B:194:GLN:HB3	2.14	0.46
1:A:56:ALA:O	1:A:202:LYS:HG3	2.15	0.46
1:B:1:MET:C	4:B:494:HOH:O	2.58	0.46
1:A:396:ALA:O	1:A:398:ASP:N	2.48	0.46
1:A:180:LEU:C	1:A:181:GLN:OE1	2.59	0.46
1:B:85:ARG:HB2	1:B:85:ARG:NH1	2.31	0.46
1:B:325:ASP:OD2	1:B:405:ARG:HB2	2.16	0.46
1:A:261:VAL:HG22	2:A:500:GLU:CG	2.46	0.46
1:B:62:ILE:HD13	1:B:142:MET:CE	2.45	0.46
1:B:116:GLY:O	1:B:120:VAL:HG23	2.16	0.46
1:A:49:ARG:N	1:A:49:ARG:CD	2.79	0.46
1:A:62:ILE:HG12	1:A:65:ALA:HB3	1.97	0.46
1:B:105:SER:O	1:B:106:HIS:ND1	2.50	0.45
1:A:296:ARG:HD3	4:A:614:HOH:O	2.17	0.45
1:A:320:VAL:HG22	1:A:329:LEU:CD1	2.46	0.45
1:B:166:ARG:O	1:B:169:SER:HB3	2.16	0.45
1:B:224:MET:HE2	1:B:224:MET:HA	1.98	0.45
1:B:264:GLY:HA2	1:B:277:VAL:O	2.16	0.45
1:B:408:VAL:HG22	1:B:440:GLU:HB3	1.99	0.45
1:A:322:ARG:CZ	1:A:399:GLU:OE2	2.64	0.45
1:A:158:GLU:OE1	1:A:158:GLU:HA	2.16	0.45
1:A:322:ARG:HG2	1:A:322:ARG:NH2	2.32	0.45
1:A:347:LEU:HD22	1:A:432:LEU:HD11	1.99	0.45
1:A:359:THR:HB	4:A:609:HOH:O	2.17	0.45
1:A:130:SER:OG	1:A:133:GLU:HG3	2.16	0.45
1:A:222:GLU:CG	1:A:224:MET:HE3	2.35	0.45
1:B:214:GLY:O	1:B:227:SER:HA	2.17	0.45
1:A:282:LEU:HA	1:A:287:ASN:O	2.16	0.45
1:A:351:ARG:HA	1:A:351:ARG:HD3	1.74	0.45
1:A:355:GLU:O	1:A:355:GLU:HG3	2.17	0.45
3:A:600:TRS:H21	4:A:507:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:CG1	1:A:65:ALA:HB3	2.46	0.45
1:A:103:ALA:C	1:A:105:SER:N	2.73	0.45
1:B:323:GLU:OE1	1:B:323:GLU:HA	2.16	0.45
1:A:110:ASN:ND2	1:A:112:MET:HB2	2.32	0.45
1:A:131:ARG:HD3	4:A:692:HOH:O	2.17	0.45
1:A:201:VAL:HG22	1:A:278:PHE:CB	2.46	0.45
1:B:223:ARG:O	1:B:224:MET:HE2	2.17	0.44
1:B:399:GLU:HB2	4:B:458:HOH:O	2.16	0.44
1:A:121:HIS:HE1	4:A:651:HOH:O	2.01	0.44
1:A:399:GLU:OE2	1:A:404:ILE:HG13	2.18	0.44
1:A:214:GLY:O	1:A:227:SER:HA	2.18	0.44
1:A:49:ARG:HG3	1:A:49:ARG:NH1	2.28	0.44
1:B:88:GLY:C	1:B:109:ASP:O	2.61	0.44
1:B:64:SER:C	1:B:66:SER:H	2.26	0.44
1:B:226:PRO:HG2	1:B:229:VAL:HB	1.99	0.44
1:B:355:GLU:H	1:B:355:GLU:CD	2.25	0.44
1:A:38:ARG:NH1	1:A:38:ARG:HG2	2.32	0.43
1:A:104:GLU:H	1:A:104:GLU:CD	2.26	0.43
1:B:106:HIS:HB3	4:B:497:HOH:O	2.18	0.43
1:B:5:ILE:HB	1:B:6:PRO:HD3	1.99	0.43
1:A:273:VAL:HG22	1:A:274:GLY:N	2.34	0.43
1:B:277:VAL:HG11	1:B:291:GLY:HA2	1.99	0.43
1:A:450:LEU:CD1	1:A:450:LEU:N	2.81	0.43
1:B:84:ASP:O	1:B:107:ARG:NH1	2.51	0.43
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.30	0.43
1:B:226:PRO:CB	3:B:600:TRS:H11	2.49	0.43
1:B:226:PRO:CA	3:B:600:TRS:H11	2.47	0.43
1:B:440:GLU:HG3	4:B:474:HOH:O	2.18	0.43
1:A:110:ASN:O	1:A:116:GLY:HA3	2.18	0.43
1:A:361:TRP:HZ3	1:A:363:ALA:HA	1.82	0.43
1:B:153:ASP:HB2	1:B:198:LEU:HD11	2.00	0.43
1:B:327:VAL:HG21	1:B:404:ILE:HD13	2.01	0.43
1:B:356:LYS:O	1:B:357:PRO:C	2.62	0.43
1:A:86:GLN:O	1:A:107:ARG:HB2	2.19	0.42
1:A:85:ARG:NH2	4:A:604:HOH:O	2.52	0.42
1:A:138:ALA:O	1:A:141:ILE:HG22	2.20	0.42
1:B:49:ARG:NE	4:B:659:HOH:O	2.52	0.42
1:B:443:ASP:HA	1:B:444:PRO:HD2	1.87	0.42
1:A:163:VAL:HB	4:A:587:HOH:O	2.18	0.42
1:B:64:SER:C	1:B:66:SER:N	2.77	0.42
1:B:105:SER:C	1:B:106:HIS:ND1	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:CD	1:B:327:VAL:HG22	2.50	0.42
1:B:365:VAL:O	1:B:367:PRO:HD3	2.19	0.42
3:A:600:TRS:H31	4:A:633:HOH:O	2.19	0.42
1:B:359:THR:HB	1:B:361:TRP:CD1	2.54	0.42
1:A:395:ALA:HA	1:A:399:GLU:HG3	2.01	0.42
1:B:261:VAL:HG22	2:B:500:GLU:CG	2.49	0.42
1:A:237:MET:CE	1:A:266:LEU:HD13	2.49	0.42
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.88	0.42
1:B:279:SER:OG	1:B:290:ARG:CD	2.68	0.42
1:A:116:GLY:O	1:A:120:VAL:HG23	2.19	0.42
1:A:222:GLU:HG3	1:A:224:MET:CE	2.36	0.42
1:B:121:HIS:HD2	1:B:194:GLN:OE1	2.03	0.42
1:B:350:LEU:O	1:B:352:THR:HG23	2.20	0.42
1:B:186:GLU:HG2	4:B:560:HOH:O	2.20	0.41
1:B:99:LEU:HD23	1:B:102:GLU:OE2	2.20	0.41
1:B:240:SER:HB3	4:B:511:HOH:O	2.20	0.41
1:B:389:HIS:HA	4:B:457:HOH:O	2.19	0.41
1:B:410:ASN:HA	1:B:442:GLU:HB2	2.01	0.41
1:A:201:VAL:CG1	1:A:276:GLY:O	2.69	0.41
1:A:223:ARG:O	1:A:224:MET:HE2	2.20	0.41
1:A:331:LEU:HD12	1:A:411:LEU:CD2	2.50	0.41
1:A:389:HIS:HE1	4:A:630:HOH:O	2.03	0.41
1:A:105:SER:O	1:A:106:HIS:HB2	2.19	0.41
1:A:226:PRO:HG2	1:A:229:VAL:HG23	2.02	0.41
1:A:368:ARG:HG2	1:A:368:ARG:HH11	1.85	0.41
1:B:329:LEU:HB3	1:B:409:LEU:HD23	2.03	0.41
1:A:62:ILE:HG21	1:A:142:MET:CE	2.27	0.41
1:B:408:VAL:HA	1:B:440:GLU:O	2.20	0.41
1:B:365:VAL:C	1:B:367:PRO:HD3	2.45	0.41
1:B:69:PHE:CZ	1:B:207:MET:HB3	2.56	0.41
1:B:361:TRP:HH2	1:B:370:GLN:HA	1.84	0.41
1:B:314:GLY:HA3	1:B:385:GLY:C	2.45	0.41
1:A:91:PRO:HB3	1:A:239:SER:O	2.19	0.41
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.83	0.41
1:B:330:HIS:CD2	1:B:410:ASN:HB3	2.56	0.41
1:A:131:ARG:CZ	1:A:186:GLU:HG3	2.51	0.40
1:A:242:MET:HG3	1:A:249:TRP:CG	2.56	0.40
1:A:419:ASP:OD1	1:A:422:ARG:NH1	2.53	0.40
1:B:322:ARG:HH21	1:B:322:ARG:HG2	1.86	0.40
1:B:363:ALA:HB1	1:B:370:GLN:OE1	2.22	0.40
1:A:88:GLY:C	1:A:109:ASP:O	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:CG1	1:A:291:GLY:HA2	2.50	0.40
1:A:355:GLU:C	1:A:357:PRO:CD	2.95	0.40
1:B:367:PRO:O	1:B:371:GLU:HG3	2.19	0.40
1:B:140:GLU:HB2	4:B:639:HOH:O	2.22	0.40
1:A:408:VAL:HG22	1:A:440:GLU:HG3	2.02	0.40

All (1) 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:B:310:ASP:O	1:B:310:ASP:O[2_655]	2.00	0.20

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	448/456 (98%)	413 (92%)	27 (6%)	8 (2%)	6	9
1	B	446/456 (98%)	411 (92%)	28 (6%)	7 (2%)	7	11
All	All	894/912 (98%)	824 (92%)	55 (6%)	15 (2%)	7	10

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	351	ARG
1	B	357	PRO
1	A	397	ARG
1	A	446	ARG
1	B	354	ALA
1	B	447	ILE
1	A	449	PRO
1	A	359	THR

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Mol	Chain	Res	Type
1	A	27	TYR
1	B	27	TYR
1	A	396	ALA
1	B	324	GLY
1	A	324	GLY
1	A	444	PRO
1	B	358	GLY

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	338/341 (99%)	332 (98%)	6 (2%)	51	73
1	B	336/341 (98%)	332 (99%)	4 (1%)	63	81
All	All	674/682 (99%)	664 (98%)	10 (2%)	57	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	135	LEU
1	A	266	LEU
1	A	356	LYS
1	A	397	ARG
1	A	450	LEU
1	B	64	SER
1	B	78	ARG
1	B	266	LEU
1	B	272	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN

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Mol	Chain	Res	Type
1	A	121	HIS
1	A	172	HIS
1	A	330	HIS
1	B	26	GLN
1	B	86	GLN
1	B	110	ASN
1	B	121	HIS
1	B	172	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](#)

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	B	500	-	7,8,9	0.94	0	4,9,11	0.81	0
3	TRS	A	600	-	7,7,7	1.97	2 (28%)	9,9,9	2.27	6 (66%)
2	GLU	A	500	-	7,8,9	0.95	0	4,9,11	0.87	0
3	TRS	B	600	-	7,7,7	2.18	2 (28%)	9,9,9	2.21	3 (33%)

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	B	500	-	-	0/6/7/9	-
3	TRS	A	600	-	-	6/9/9/9	-
2	GLU	A	500	-	-	3/6/7/9	-
3	TRS	B	600	-	-	6/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	TRS	C2-C	-4.98	1.39	1.53
3	A	600	TRS	C2-C	-4.34	1.41	1.53
3	A	600	TRS	O1-C1	-2.40	1.34	1.42
3	B	600	TRS	O1-C1	-2.28	1.35	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	TRS	O3-C3-C	4.96	124.71	110.88
3	A	600	TRS	O3-C3-C	4.25	122.72	110.88
3	B	600	TRS	C3-C-N	3.07	116.00	108.17
3	A	600	TRS	C3-C-C1	-2.53	103.91	110.66
3	A	600	TRS	C3-C-N	2.50	114.54	108.17
3	A	600	TRS	C2-C-C1	-2.45	104.13	110.66
3	A	600	TRS	C3-C-C2	2.14	116.35	110.66
3	B	600	TRS	C2-C-C1	-2.10	105.06	110.66
3	A	600	TRS	O2-C2-C	2.04	116.56	110.88

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	TRS	C2-C-C1-O1
3	A	600	TRS	C3-C-C1-O1
3	A	600	TRS	C1-C-C3-O3
3	A	600	TRS	C2-C-C3-O3
3	A	600	TRS	N-C-C3-O3
3	B	600	TRS	C2-C-C1-O1
3	B	600	TRS	C3-C-C1-O1

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Mol	Chain	Res	Type	Atoms
3	B	600	TRS	C1-C-C3-O3
3	B	600	TRS	C2-C-C3-O3
3	B	600	TRS	N-C-C3-O3
3	A	600	TRS	N-C-C1-O1
3	B	600	TRS	N-C-C1-O1
2	A	500	GLU	C-CA-CB-CG
2	A	500	GLU	OE2-CD-CG-CB
2	A	500	GLU	OE1-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	GLU	7	0
3	A	600	TRS	2	0
2	A	500	GLU	3	0
3	B	600	TRS	5	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	450/456 (98%)	-0.01	23 (5%) 33 30	17, 34, 78, 110	0
1	B	448/456 (98%)	0.01	19 (4%) 40 36	17, 36, 74, 105	0
All	All	898/912 (98%)	0.00	42 (4%) 36 32	17, 35, 75, 110	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	GLY	5.7
1	A	450	LEU	5.7
1	B	105	SER	4.8
1	B	448	LEU	4.4
1	A	399	GLU	4.2
1	A	351	ARG	4.1
1	A	357	PRO	4.0
1	B	324	GLY	4.0
1	A	354	ALA	3.4
1	A	359	THR	3.4
1	A	445	GLU	3.0
1	B	359	THR	3.0
1	A	136	ASP	3.0
1	B	447	ILE	3.0
1	A	322	ARG	3.0
1	B	446	ARG	3.0
1	B	355	GLU	2.9
1	B	106	HIS	2.8
1	A	325	ASP	2.8
1	A	397	ARG	2.7
1	A	448	LEU	2.7
1	A	402	GLY	2.6
1	A	358	GLY	2.6
1	A	400	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	353	GLY	2.4
1	A	105	SER	2.3
1	A	356	LYS	2.3
1	B	357	PRO	2.3
1	A	398	ASP	2.3
1	B	401	ASP	2.2
1	B	400	ASN	2.2
1	A	360	GLY	2.2
1	B	102	GLU	2.2
1	B	325	ASP	2.2
1	A	396	ALA	2.1
1	B	136	ASP	2.1
1	A	361	TRP	2.1
1	B	360	GLY	2.1
1	B	28	ILE	2.1
1	A	437	VAL	2.1
1	B	437	VAL	2.0
1	B	432	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TRS	B	600	8/8	0.55	0.26	69,72,75,75	0
3	TRS	A	600	8/8	0.63	0.25	74,78,80,83	0
2	GLU	B	500	9/10	0.84	0.13	34,37,44,44	0
2	GLU	A	500	9/10	0.85	0.12	31,34,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.