



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:11 PM EDT

PDB ID : 4Z1Y / pdb_00004z1y
Title : Thermostable enolase from *Chloroflexus aurantiacus* with substrate 2-phosphoglycerate
Authors : Zadvornyy, O.A.; Peters, J.W.
Deposited on : 2015-03-27
Resolution : 2.53 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

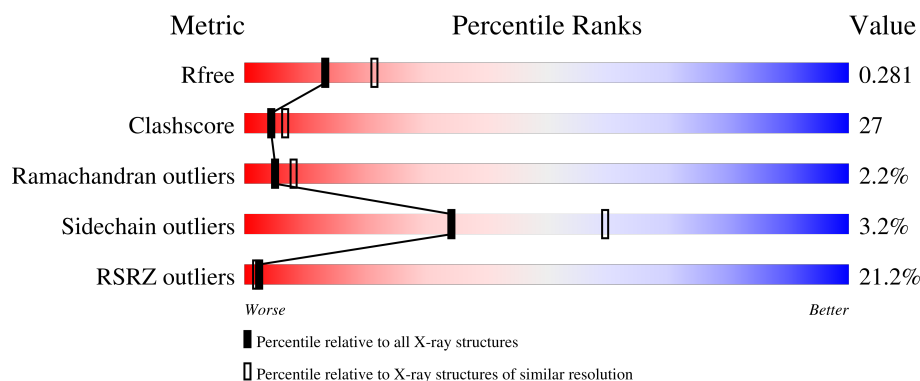
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	426	
1	B	426	

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
3	2PG	B	502[B]	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6466 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.

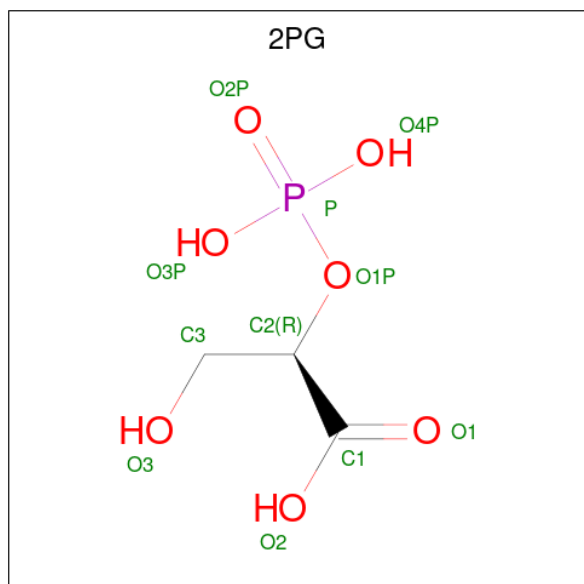
- Molecule 1 is a protein called Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	2	7	0
			3250	2037	572	633	8			
1	B	419	Total	C	N	O	S	0	0	0
			3169	1987	559	615	8			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (CCD ID: 2PG) (formula: C₃H₇O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	1
			11	3	7	1		
3	B	1	Total	C	O	P	0	1
			11	3	7	1		

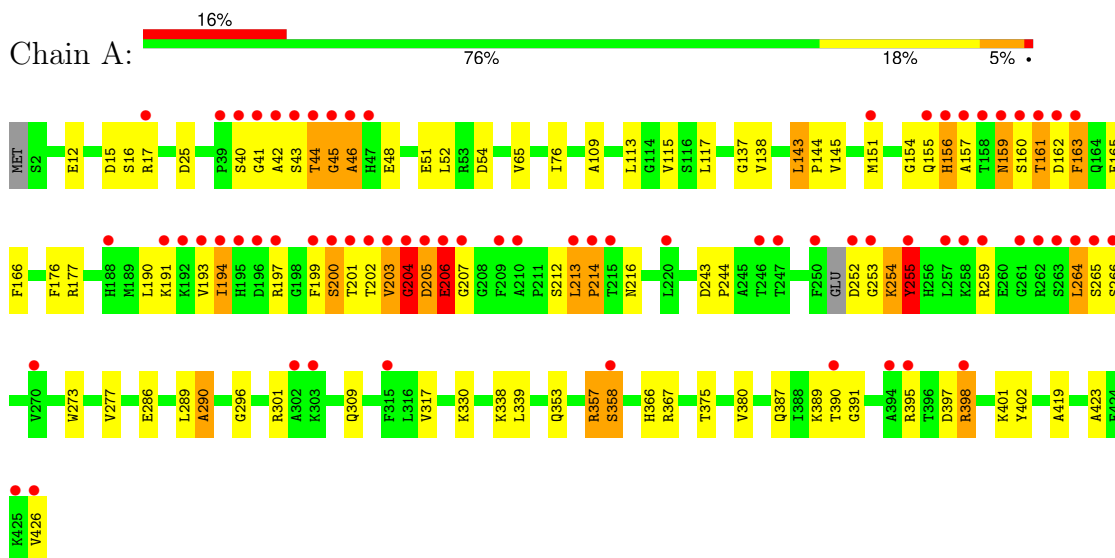
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	12	Total	O	0	0
			12	12		

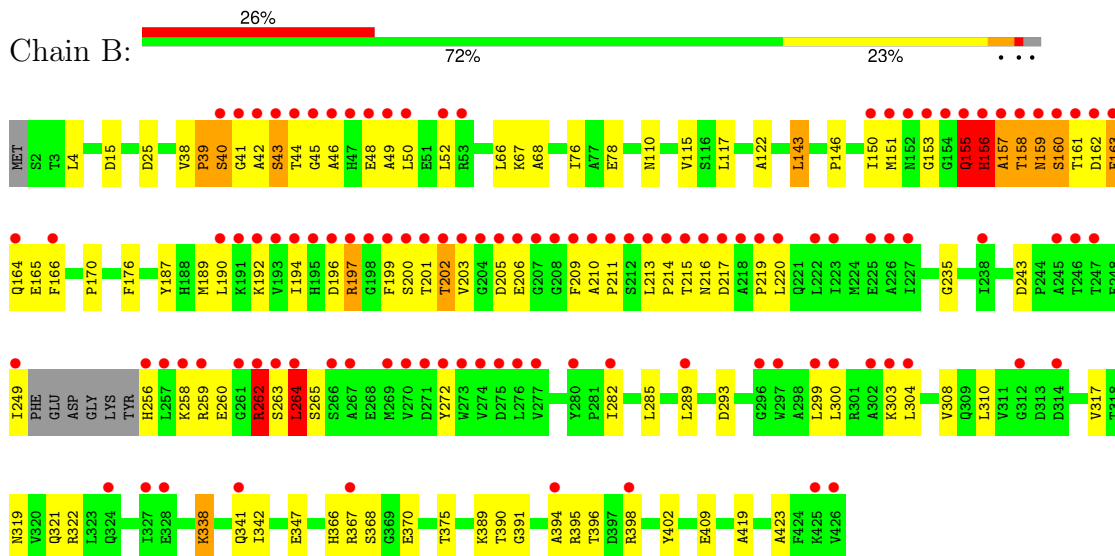
3 Residue-property plots [i](#)

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: Enolase



• Molecule 1: Enolase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.32Å 146.32Å 101.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.70 – 2.53 37.70 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.70-2.53) 99.9 (37.70-2.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.1, REFMAC	Depositor
R, R_{free}	0.214 , 0.252 0.247 , 0.281	Depositor DCC
R_{free} test set	1794 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2PG

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	0.82	1/3300 (0.0%)	1.37	26/4471 (0.6%)
1	B	1.03	5/3217 (0.2%)	1.56	35/4360 (0.8%)
All	All	0.93	6/6517 (0.1%)	1.47	61/8831 (0.7%)

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	1
1	B	0	4
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	THR	C-N	-20.34	1.04	1.33
1	B	155	GLN	C-N	-17.38	1.10	1.33
1	B	264	LEU	C-N	16.64	1.56	1.33
1	B	262	ARG	C-N	-14.51	1.12	1.33
1	A	204	GLY	C-N	-7.66	1.23	1.33
1	B	317	VAL	CA-C	5.62	1.59	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	THR	O-C-N	-20.62	95.48	123.11
1	B	262	ARG	CB-CA-C	-18.03	88.14	111.40
1	B	265	SER	N-CA-CB	17.92	140.97	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	ASN	N-CA-CB	-16.11	83.61	109.87
1	B	155	GLN	O-C-N	-15.70	101.70	122.59
1	B	262	ARG	O-C-N	-13.37	101.17	121.89
1	B	159	ASN	N-CA-C	13.00	129.15	109.25
1	A	204	GLY	O-C-N	-12.39	113.05	122.71
1	B	155	GLN	N-CA-C	11.91	136.17	110.80
1	B	156	HIS	N-CA-CB	-11.59	88.14	110.63
1	B	155	GLN	CB-CA-C	-11.40	87.74	110.42
1	B	264	LEU	CB-CA-C	10.27	130.85	110.42
1	B	262	ARG	CA-C-N	9.88	136.04	121.72
1	B	262	ARG	C-N-CA	9.88	136.04	121.72
1	A	264	LEU	CB-CA-C	9.06	128.45	110.42
1	B	158	THR	N-CA-C	-8.96	95.69	109.85
1	B	263	SER	N-CA-CB	-8.88	95.39	109.87
1	B	264	LEU	N-CA-C	-8.34	93.03	110.80
1	A	357	ARG	N-CA-C	-8.27	97.55	109.96
1	A	205	ASP	N-CA-C	8.18	128.23	110.80
1	B	158	THR	CA-C-N	7.77	132.99	121.72
1	B	158	THR	C-N-CA	7.77	132.99	121.72
1	B	15	ASP	CA-CB-CG	7.27	119.87	112.60
1	B	158	THR	CB-CA-C	-7.02	96.04	109.66
1	A	290	ALA	CA-C-N	6.52	130.60	120.82
1	A	290	ALA	C-N-CA	6.52	130.60	120.82
1	A	338	LYS	CA-C-N	6.49	130.55	120.82
1	A	338	LYS	C-N-CA	6.49	130.55	120.82
1	B	265	SER	N-CA-C	-6.39	93.12	111.00
1	A	145	VAL	N-CA-C	-6.22	101.47	107.76
1	B	391	GLY	N-CA-C	6.09	120.70	112.17
1	A	255	TYR	CB-CA-C	5.97	122.30	110.42
1	A	137	GLY	CA-C-N	5.84	129.70	120.47
1	A	137	GLY	C-N-CA	5.84	129.70	120.47
1	A	206	GLU	N-CA-C	-5.83	105.83	113.12
1	A	25	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	204	GLY	N-CA-C	-5.66	102.76	111.98
1	B	338	LYS	CA-C-N	5.55	128.03	120.54
1	B	338	LYS	C-N-CA	5.55	128.03	120.54
1	B	260	GLU	N-CA-C	-5.44	106.65	113.72
1	A	398	ARG	CA-C-N	5.40	128.14	120.53
1	A	398	ARG	C-N-CA	5.40	128.14	120.53
1	B	264	LEU	CA-C-N	5.35	131.33	121.70
1	B	264	LEU	C-N-CA	5.35	131.33	121.70
1	A	15	ASP	CA-CB-CG	5.34	117.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	LEU	CA-C-N	5.33	132.45	122.74
1	A	264	LEU	C-N-CA	5.33	132.45	122.74
1	B	143	LEU	CD1-CG-CD2	5.32	122.51	110.80
1	A	54	ASP	N-CA-C	5.32	117.16	111.36
1	B	122	ALA	CA-C-N	5.29	127.81	120.29
1	B	122	ALA	C-N-CA	5.29	127.81	120.29
1	B	293	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	235	GLY	CA-C-N	5.26	127.33	120.28
1	B	235	GLY	C-N-CA	5.26	127.33	120.28
1	B	25	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	216	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	109	ALA	CA-C-N	5.11	127.55	120.29
1	A	109	ALA	C-N-CA	5.11	127.55	120.29
1	B	196	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	205	ASP	N-CA-CB	-5.07	101.93	110.49
1	A	143	LEU	CD1-CG-CD2	5.01	121.82	110.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	GLY	Mainchain
1	B	155	GLN	Mainchain
1	B	158	THR	Mainchain
1	B	262	ARG	Mainchain
1	B	264	LEU	Mainchain

5.2 Too-close contacts [i](#)

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	3250	0	3244	132	0
1	B	3169	0	3171	235	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	4	0	0
3	B	11	0	4	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	11	0	0	0	0
4	B	12	0	0	0	0
All	All	6466	0	6423	342	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 27.

All (342) 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:209:PHE:CD2	1:B:211:PRO:HD3	1.46	1.46
1:B:156:HIS:N	1:B:157:ALA:CB	1.77	1.45
1:B:161:THR:CG2	1:B:216:ASN:OD1	1.73	1.36
1:B:156:HIS:N	1:B:157:ALA:HB2	1.01	1.31
1:A:42[A]:ALA:O	1:A:51:GLU:CG	1.78	1.29
1:B:156:HIS:CB	1:B:157:ALA:HB2	1.62	1.27
1:B:41:GLY:CA	1:B:367:ARG:HD3	1.64	1.26
1:A:395:ARG:NH1	1:B:395:ARG:CG	2.02	1.23
1:B:366:HIS:CD2	1:B:390:THR:HA	1.75	1.22
1:A:254:LYS:CB	1:A:264:LEU:O	1.88	1.20
1:A:254:LYS:HB3	1:A:264:LEU:O	1.06	1.18
1:A:160:SER:O	1:A:161:THR:CG2	1.92	1.17
1:A:160:SER:O	1:A:161:THR:HG22	1.02	1.17
1:B:262:ARG:NH1	1:B:272:TYR:CD2	2.12	1.17
1:A:17:ARG:NH1	1:A:205:ASP:OD2	1.80	1.15
1:B:156:HIS:CA	1:B:157:ALA:HB2	1.76	1.15
1:B:161:THR:HG23	1:B:216:ASN:OD1	1.32	1.14
1:B:156:HIS:HB3	1:B:157:ALA:HA	1.23	1.12
1:B:390:THR:O	1:B:398:ARG:HD2	1.49	1.13
1:B:41:GLY:HA3	1:B:367:ARG:HD3	1.16	1.12
1:A:395:ARG:NH1	1:B:395:ARG:HG2	1.60	1.12
1:B:44:THR:HB	1:B:45:GLY:CA	1.78	1.12
1:A:17:ARG:CZ	1:A:205:ASP:OD2	1.96	1.11
1:A:42[A]:ALA:O	1:A:51:GLU:HG2	0.93	1.11
1:B:209:PHE:CD2	1:B:211:PRO:CD	2.33	1.10
1:A:254:LYS:HG3	1:A:265:SER:HA	1.25	1.10
1:B:156:HIS:HB3	1:B:157:ALA:CA	1.79	1.10
1:B:209:PHE:HE2	1:B:211:PRO:CB	1.63	1.09
1:B:156:HIS:CB	1:B:157:ALA:CB	2.30	1.08
1:B:156:HIS:HB2	1:B:157:ALA:HB2	1.28	1.08
1:A:395:ARG:HH11	1:B:395:ARG:CG	1.63	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:HH22	1:B:203:VAL:HG21	1.18	1.06
1:A:395:ARG:NH2	1:B:203:VAL:HG21	1.71	1.04
1:B:304:LEU:HD13	1:B:308:VAL:CG2	1.86	1.04
1:B:366:HIS:HD2	1:B:390:THR:CA	1.70	1.04
1:B:213:LEU:HD13	1:B:219:PRO:HG3	1.38	1.03
1:A:395:ARG:HH11	1:B:395:ARG:HG2	0.90	1.03
1:B:262:ARG:NH1	1:B:272:TYR:HD2	1.48	1.03
1:A:395:ARG:NH2	1:B:203:VAL:CG2	2.22	1.03
1:B:44:THR:HB	1:B:45:GLY:HA2	1.35	1.02
1:B:370:GLU:CG	1:B:398:ARG:HH12	1.72	1.02
1:B:258:LYS:HA	1:B:259:ARG:HD2	1.40	1.01
1:B:366:HIS:HD2	1:B:390:THR:HA	0.90	1.01
1:B:41:GLY:N	1:B:367:ARG:HD3	1.76	1.00
1:B:41:GLY:HA3	1:B:367:ARG:CD	1.91	0.99
1:B:44:THR:HB	1:B:45:GLY:C	1.86	0.99
1:A:395:ARG:HH22	1:B:203:VAL:CG2	1.74	0.97
1:B:370:GLU:CB	1:B:398:ARG:HH12	1.77	0.96
1:B:209:PHE:CE2	1:B:211:PRO:CD	2.48	0.96
1:B:304:LEU:HD13	1:B:308:VAL:CB	1.93	0.96
1:B:304:LEU:CD1	1:B:308:VAL:HB	1.95	0.96
1:B:341:GLN:NE2	1:B:367:ARG:HH22	1.64	0.95
1:B:209:PHE:CE2	1:B:211:PRO:HB3	2.02	0.94
1:A:252:ASP:HB2	1:A:253:GLY:HA2	1.48	0.94
1:B:367:ARG:HG3	3:B:502[B]:2PG:O2P	1.67	0.94
1:A:395:ARG:NH1	1:B:395:ARG:HG3	1.80	0.93
1:B:213:LEU:CD1	1:B:219:PRO:HG3	1.98	0.93
1:B:209:PHE:HE2	1:B:211:PRO:HB3	1.32	0.92
1:B:209:PHE:CE2	1:B:211:PRO:CB	2.53	0.92
1:B:341:GLN:HE21	1:B:367:ARG:HH22	1.01	0.92
1:B:41:GLY:N	1:B:367:ARG:CD	2.32	0.91
1:B:209:PHE:CE2	1:B:211:PRO:HD3	2.05	0.91
1:B:44:THR:CB	1:B:45:GLY:C	2.43	0.91
1:B:338:LYS:HD3	1:B:341:GLN:NE2	1.85	0.90
1:B:304:LEU:HD13	1:B:308:VAL:HB	1.50	0.90
1:B:209:PHE:HD2	1:B:211:PRO:CD	1.75	0.90
1:B:161:THR:HG21	1:B:216:ASN:OD1	1.71	0.89
1:A:160:SER:HB2	1:A:212:SER:HA	1.54	0.89
1:B:44:THR:CG2	1:B:48:GLU:CG	2.51	0.89
1:B:156:HIS:CB	1:B:157:ALA:CA	2.46	0.89
1:B:370:GLU:HG3	1:B:398:ARG:NH1	1.88	0.89
1:B:370:GLU:CG	1:B:398:ARG:NH1	2.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLY:CA	1:B:367:ARG:CD	2.50	0.88
1:B:197:ARG:CG	1:B:199:PHE:HE2	1.87	0.88
1:B:156:HIS:HB2	1:B:157:ALA:CB	1.98	0.88
1:B:209:PHE:HE2	1:B:211:PRO:CA	1.87	0.88
1:A:252:ASP:HB2	1:A:253:GLY:CA	2.05	0.87
1:A:395:ARG:HH12	1:B:395:ARG:HG3	1.35	0.86
1:B:44:THR:HG23	1:B:48:GLU:CD	2.00	0.86
1:B:342:ILE:HD11	1:B:347:GLU:HB3	1.57	0.86
1:B:197:ARG:CG	1:B:199:PHE:CE2	2.59	0.86
1:A:254:LYS:CG	1:A:265:SER:HA	2.03	0.86
1:B:338:LYS:CD	1:B:341:GLN:NE2	2.39	0.86
1:B:44:THR:HG22	1:B:45:GLY:O	1.75	0.85
1:B:156:HIS:N	1:B:157:ALA:HB3	1.90	0.85
1:A:390:THR:HG22	1:A:390:THR:O	1.77	0.85
1:B:262:ARG:HH12	1:B:272:TYR:HD2	1.06	0.85
1:B:304:LEU:HD13	1:B:308:VAL:HG21	1.57	0.85
1:B:42:ALA:HB1	1:B:43:SER:HA	1.57	0.84
1:A:202:THR:O	1:A:203:VAL:HG13	1.77	0.84
1:B:44:THR:CG2	1:B:45:GLY:O	2.26	0.84
1:B:205:ASP:O	1:B:395:ARG:NH1	2.10	0.84
1:B:197:ARG:HG3	1:B:199:PHE:CE2	2.12	0.83
1:A:309:GLN:HE22	1:A:387:GLN:HE22	1.26	0.83
1:B:44:THR:CB	1:B:45:GLY:O	2.26	0.83
1:A:366:HIS:ND1	1:A:390:THR:HA	1.95	0.82
1:B:44:THR:CA	1:B:45:GLY:C	2.48	0.82
1:B:370:GLU:HB2	1:B:398:ARG:HH12	1.41	0.82
1:A:206:GLU:HA	1:A:398:ARG:HE	1.43	0.82
1:B:44:THR:HB	1:B:45:GLY:O	1.79	0.82
1:B:44:THR:HA	1:B:45:GLY:C	2.04	0.81
1:B:209:PHE:CE2	1:B:211:PRO:N	2.48	0.81
1:B:390:THR:O	1:B:398:ARG:CD	2.28	0.81
1:A:12:GLU:HG3	1:A:65:VAL:HG12	1.62	0.81
1:A:366:HIS:ND1	1:A:389:LYS:O	2.12	0.81
1:B:342:ILE:CD1	1:B:347:GLU:HB3	2.10	0.81
1:B:48:GLU:O	1:B:50:LEU:HD22	1.82	0.79
1:B:197:ARG:HG3	1:B:199:PHE:CD2	2.18	0.79
1:A:206:GLU:HA	1:A:398:ARG:NE	1.95	0.79
1:A:160:SER:HB2	1:A:212:SER:CA	2.13	0.79
1:A:202:THR:O	1:A:203:VAL:CG1	2.30	0.79
1:B:262:ARG:NH1	1:B:272:TYR:CE2	2.50	0.79
1:A:202:THR:HB	1:B:202:THR:OG1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:NH2	1:B:203:VAL:HG22	1.97	0.77
1:B:338:LYS:HB2	1:B:341:GLN:OE1	1.85	0.77
1:B:366:HIS:CD2	1:B:390:THR:CA	2.54	0.77
1:B:40:SER:C	1:B:367:ARG:HD2	2.09	0.76
1:A:254:LYS:O	1:A:255:TYR:HB2	1.85	0.76
1:A:45[B]:GLY:O	1:A:46[B]:ALA:HB3	1.86	0.76
1:B:197:ARG:NH2	1:B:199:PHE:CZ	2.54	0.76
1:A:154:GLY:H	1:A:161:THR:HG23	1.51	0.75
1:A:160:SER:HB3	1:A:213:LEU:O	1.86	0.75
1:B:44:THR:CB	1:B:45:GLY:CA	2.56	0.74
1:A:160:SER:C	1:A:161:THR:HG22	2.09	0.73
1:A:202:THR:CB	1:B:202:THR:HG21	2.19	0.72
1:B:44:THR:HG22	1:B:48:GLU:HG2	1.71	0.72
1:B:42:ALA:H	1:B:367:ARG:NH1	1.88	0.72
1:B:338:LYS:HD3	1:B:367:ARG:NH2	2.03	0.72
1:B:209:PHE:CE2	1:B:211:PRO:CA	2.71	0.72
1:A:203:VAL:HG23	1:A:203:VAL:O	1.90	0.72
1:A:252:ASP:CB	1:A:253:GLY:CA	2.68	0.71
1:A:390:THR:O	1:A:398:ARG:HD2	1.90	0.71
1:B:197:ARG:CD	1:B:199:PHE:HE2	2.02	0.71
1:B:197:ARG:NH2	1:B:199:PHE:CE2	2.58	0.71
1:B:338:LYS:HB2	1:B:341:GLN:CD	2.16	0.71
1:B:258:LYS:HG2	1:B:259:ARG:CD	2.21	0.71
1:B:341:GLN:NE2	1:B:367:ARG:NH2	2.37	0.71
1:A:252:ASP:CB	1:A:253:GLY:HA2	2.18	0.71
1:A:357:ARG:O	1:A:358:SER:OG	2.09	0.70
1:B:42:ALA:CB	1:B:43:SER:HA	2.16	0.70
1:B:200:SER:O	1:B:209:PHE:CE1	2.44	0.70
1:B:155:GLN:C	1:B:157:ALA:HB2	1.96	0.70
1:B:42:ALA:H	1:B:367:ARG:HH11	1.36	0.70
1:A:202:THR:HB	1:B:202:THR:HG21	1.73	0.70
1:B:341:GLN:HE21	1:B:367:ARG:NH2	1.85	0.70
1:B:42:ALA:HB1	1:B:43:SER:CA	2.23	0.69
1:B:256:HIS:NE2	1:B:264:LEU:HD23	2.08	0.69
1:B:41:GLY:N	1:B:367:ARG:HD2	2.08	0.69
1:B:338:LYS:CD	1:B:341:GLN:CD	2.66	0.68
1:A:43[B]:SER:C	1:A:44[B]:THR:HG1	2.01	0.68
1:A:390:THR:O	1:A:390:THR:CG2	2.41	0.68
1:B:200:SER:O	1:B:209:PHE:HE1	1.77	0.68
1:A:202:THR:C	1:A:203:VAL:HG13	2.19	0.68
1:A:45[B]:GLY:O	1:A:46[B]:ALA:CB	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PHE:HD2	1:B:166:PHE:CZ	2.13	0.66
1:B:44:THR:CB	1:B:45:GLY:HA2	2.20	0.66
1:A:254:LYS:HG3	1:A:265:SER:CA	2.14	0.66
1:A:12:GLU:HG3	1:A:65:VAL:CG1	2.25	0.65
1:B:338:LYS:HD2	1:B:341:GLN:NE2	2.12	0.65
1:A:395:ARG:HH12	1:B:395:ARG:CG	1.89	0.65
1:B:44:THR:CG2	1:B:48:GLU:CD	2.69	0.65
1:A:154:GLY:O	1:A:157:ALA:HB3	1.96	0.65
1:A:203:VAL:HG12	1:A:207:GLY:O	1.96	0.65
1:A:160:SER:HB3	1:A:213:LEU:N	2.12	0.64
1:B:41:GLY:HA3	1:B:367:ARG:CG	2.27	0.64
1:B:44:THR:CG2	1:B:48:GLU:HG2	2.24	0.64
1:B:143:LEU:HD13	1:B:409:GLU:HB2	1.79	0.64
1:B:209:PHE:CD2	1:B:210:ALA:N	2.66	0.64
1:B:48:GLU:O	1:B:50:LEU:CD2	2.46	0.64
1:A:202:THR:HB	1:B:202:THR:CG2	2.29	0.63
1:A:191:LYS:HE3	1:A:201:THR:HG21	1.80	0.63
1:A:44[B]:THR:O	1:A:45[B]:GLY:C	2.42	0.63
1:B:213:LEU:HD13	1:B:219:PRO:CG	2.25	0.62
1:B:258:LYS:HG2	1:B:259:ARG:HD3	1.81	0.62
1:B:258:LYS:HG2	1:B:259:ARG:HD2	1.81	0.62
1:B:338:LYS:HD3	1:B:341:GLN:CD	2.24	0.62
1:B:370:GLU:CB	1:B:398:ARG:NH1	2.59	0.62
1:B:44:THR:CG2	1:B:48:GLU:HG3	2.30	0.62
1:B:153:GLY:HA2	1:B:160:SER:OG	2.00	0.62
1:B:366:HIS:CD2	1:B:390:THR:C	2.78	0.62
1:B:197:ARG:HD2	1:B:199:PHE:CE2	2.35	0.61
1:A:202:THR:HB	1:B:202:THR:CB	2.31	0.61
1:A:155:GLN:C	1:A:157:ALA:H	2.09	0.61
1:B:367:ARG:NH1	3:B:502[B]:2PG:O4P	2.33	0.61
1:A:177:ARG:HH22	1:B:66:LEU:HD21	1.66	0.60
1:B:76:ILE:HG21	1:B:115:VAL:HG21	1.83	0.60
1:B:202:THR:CG2	1:B:203:VAL:N	2.64	0.60
1:A:202:THR:HA	1:B:202:THR:HG21	1.82	0.60
1:B:52:LEU:HD21	1:B:67:LYS:HB3	1.83	0.59
1:A:165:GLU:HG3	1:A:243:ASP:HB3	1.85	0.59
1:B:161:THR:HG23	1:B:216:ASN:CG	2.23	0.59
1:B:44:THR:HG21	1:B:48:GLU:HG3	1.85	0.59
1:B:209:PHE:CE2	1:B:211:PRO:CG	2.85	0.59
1:B:256:HIS:NE2	1:B:264:LEU:CD2	2.66	0.58
1:B:304:LEU:CD1	1:B:308:VAL:CB	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:THR:CA	1:B:202:THR:HG21	2.34	0.58
1:B:159:ASN:CG	1:B:159:ASN:O	2.46	0.58
1:B:197:ARG:HH21	1:B:199:PHE:HZ	1.48	0.58
1:B:151:MET:SD	1:B:219:PRO:HB3	2.44	0.58
1:B:39:PRO:O	1:B:40:SER:HB3	2.02	0.58
1:B:209:PHE:HE2	1:B:211:PRO:CG	2.16	0.57
1:B:44:THR:HA	1:B:46:ALA:CB	2.33	0.57
1:A:395:ARG:CZ	1:B:203:VAL:HG21	2.33	0.57
1:B:202:THR:HG23	1:B:203:VAL:N	2.20	0.57
1:A:254:LYS:O	1:A:255:TYR:CB	2.51	0.57
1:B:209:PHE:HD2	1:B:211:PRO:HD3	0.78	0.57
1:B:44:THR:HA	1:B:46:ALA:N	2.21	0.56
1:A:17:ARG:NH2	1:A:205:ASP:OD2	2.35	0.56
1:A:206:GLU:HA	1:A:398:ARG:CZ	2.35	0.56
1:A:254:LYS:HD2	1:A:266:SER:H	1.70	0.56
1:A:194:ILE:HG23	1:A:199:PHE:HB2	1.87	0.56
1:B:155:GLN:C	1:B:157:ALA:CB	2.61	0.55
1:B:197:ARG:NH2	1:B:199:PHE:HZ	2.04	0.55
1:B:258:LYS:HA	1:B:259:ARG:CD	2.26	0.55
1:B:341:GLN:HG3	1:B:367:ARG:HH21	1.70	0.55
1:B:163:PHE:HD2	1:B:166:PHE:HZ	1.53	0.55
1:B:165:GLU:HB2	1:B:243:ASP:HB3	1.88	0.55
1:B:285:LEU:HD23	1:B:310:LEU:HD22	1.88	0.54
1:B:338:LYS:HD2	1:B:341:GLN:CD	2.31	0.54
1:A:160:SER:O	1:A:161:THR:CB	2.55	0.54
1:A:205:ASP:O	1:A:398:ARG:NH2	2.40	0.54
1:B:190:LEU:HG	1:B:194:ILE:HD12	1.88	0.54
1:B:143:LEU:HD11	1:B:409:GLU:HA	1.90	0.54
1:B:40:SER:C	1:B:367:ARG:CD	2.73	0.54
1:A:214:PRO:HA	1:A:259:ARG:HH21	1.73	0.54
1:A:40[A]:SER:O	1:A:367:ARG:HB3	2.08	0.53
1:B:143:LEU:CD1	1:B:409:GLU:HB2	2.38	0.53
1:A:160:SER:CB	1:A:213:LEU:N	2.72	0.53
1:B:43:SER:O	1:B:44:THR:OG1	2.25	0.53
1:A:76:ILE:HG21	1:A:115:VAL:HG21	1.91	0.53
1:B:341:GLN:CG	1:B:367:ARG:NH2	2.72	0.53
1:B:215:THR:HG22	1:B:217:ASP:H	1.73	0.53
1:A:390:THR:HG21	1:A:401:LYS:HB2	1.91	0.52
1:B:143:LEU:CD1	1:B:409:GLU:HG3	2.40	0.52
1:B:143:LEU:CD1	1:B:409:GLU:CB	2.88	0.51
1:B:197:ARG:HH21	1:B:199:PHE:HE2	1.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:HD12	1:B:308:VAL:HB	1.84	0.51
1:B:143:LEU:CD1	1:B:409:GLU:CG	2.89	0.51
1:B:42:ALA:O	1:B:367:ARG:NH1	2.43	0.51
1:B:209:PHE:HE2	1:B:211:PRO:N	1.94	0.51
1:A:254:LYS:CG	1:A:264:LEU:O	2.58	0.50
1:A:395:ARG:NH1	1:B:395:ARG:CD	2.73	0.50
1:B:197:ARG:O	1:B:197:ARG:HD3	2.11	0.50
1:B:44:THR:HA	1:B:46:ALA:HB3	1.93	0.50
1:A:162:ASP:O	1:A:163:PHE:O	2.30	0.50
1:B:38:VAL:HG11	1:B:110:ASN:HA	1.94	0.49
1:B:44:THR:HG23	1:B:48:GLU:OE1	2.12	0.49
1:B:370:GLU:HB2	1:B:398:ARG:NH1	2.19	0.49
1:A:254:LYS:HD2	1:A:266:SER:N	2.27	0.49
1:B:197:ARG:CD	1:B:197:ARG:O	2.60	0.49
1:A:151:MET:HB3	1:A:166:PHE:HB2	1.94	0.49
1:A:395:ARG:HG2	1:B:395:ARG:HE	1.76	0.49
1:A:42[A]:ALA:O	1:A:51:GLU:CD	2.49	0.49
1:A:206:GLU:HA	1:A:398:ARG:NH2	2.28	0.49
1:B:159:ASN:O	1:B:159:ASN:OD1	2.30	0.49
1:B:209:PHE:HE2	1:B:211:PRO:CD	2.07	0.49
1:A:254:LYS:CD	1:A:265:SER:HA	2.43	0.49
1:A:16:SER:O	1:B:394:ALA:O	2.30	0.48
1:A:200:SER:OG	1:A:201:THR:N	2.46	0.48
1:B:197:ARG:CD	1:B:199:PHE:CE2	2.85	0.48
1:B:319:ASN:HD22	1:B:322:ARG:HG2	1.78	0.48
1:A:206:GLU:O	1:A:398:ARG:HG3	2.14	0.48
1:A:144:PRO:HG3	1:A:380:VAL:HG11	1.96	0.47
1:B:366:HIS:CD2	1:B:389:LYS:O	2.67	0.47
1:A:203:VAL:HB	1:A:207:GLY:HA2	1.96	0.47
1:A:160:SER:CB	1:A:212:SER:C	2.87	0.47
1:A:203:VAL:O	1:A:203:VAL:CG2	2.61	0.47
1:B:258:LYS:CA	1:B:259:ARG:HD2	2.29	0.47
1:B:419:ALA:HB1	1:B:423:ALA:HB2	1.95	0.47
1:A:390:THR:O	1:A:398:ARG:CD	2.60	0.47
1:A:255:TYR:OH	1:A:290:ALA:N	2.39	0.47
1:A:46[B]:ALA:O	1:A:317:VAL:HG11	2.15	0.47
1:A:253:GLY:O	1:A:254:LYS:HE2	2.14	0.46
1:B:52:LEU:HD23	1:B:68:ALA:N	2.30	0.46
1:B:338:LYS:CD	1:B:341:GLN:HE22	2.25	0.46
1:B:338:LYS:HD2	1:B:341:GLN:HE22	1.78	0.46
1:B:289:LEU:HD12	1:B:300:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:CG	3:B:502[B]:2PG:O2P	2.51	0.46
1:A:44[B]:THR:O	1:A:45[B]:GLY:O	2.34	0.45
1:A:46[B]:ALA:N	1:A:48:GLU:OE1	2.37	0.45
1:A:397:ASP:HB3	1:B:396:THR:OG1	2.16	0.45
1:B:164:GLN:HB3	1:B:243:ASP:O	2.17	0.45
1:B:319:ASN:HB3	1:B:322:ARG:HG2	1.97	0.45
1:A:113:LEU:HD11	1:A:339:LEU:HG	1.99	0.45
1:B:215:THR:HG22	1:B:216:ASN:N	2.32	0.45
1:A:391:GLY:HA3	1:A:398:ARG:HD2	1.98	0.44
1:B:189:MET:HA	1:B:192:LYS:HD2	1.99	0.44
1:B:341:GLN:CG	1:B:367:ARG:HH21	2.30	0.44
1:A:154:GLY:N	1:A:163:PHE:O	2.51	0.44
1:A:252:ASP:HB2	1:A:253:GLY:HA3	1.93	0.44
1:B:367:ARG:HG2	1:B:368:SER:H	1.83	0.44
1:B:206:GLU:OE2	3:B:502[B]:2PG:C3	2.65	0.44
1:B:367:ARG:O	1:B:398:ARG:NH2	2.49	0.44
1:B:367:ARG:HG2	1:B:368:SER:N	2.32	0.44
1:A:254:LYS:HD2	1:A:265:SER:HA	2.00	0.44
1:A:397:ASP:OD1	1:A:398:ARG:HG2	2.18	0.44
1:B:256:HIS:CD2	1:B:264:LEU:HD23	2.51	0.44
1:B:48:GLU:HG2	1:B:48:GLU:H	1.63	0.43
1:B:209:PHE:CG	1:B:210:ALA:N	2.85	0.43
1:B:390:THR:C	1:B:398:ARG:HD2	2.36	0.43
1:B:143:LEU:HD12	1:B:409:GLU:HG3	2.01	0.43
1:A:117:LEU:HD22	1:A:375:THR:HG21	2.01	0.43
1:B:163:PHE:CD2	1:B:166:PHE:HZ	2.34	0.43
1:A:203:VAL:C	1:A:204:GLY:O	2.60	0.43
1:A:419:ALA:HB1	1:A:423:ALA:HB2	2.00	0.43
1:B:49:ALA:C	1:B:50:LEU:HD22	2.43	0.43
1:A:176:PHE:HZ	1:A:402:TYR:HD1	1.67	0.43
1:B:220:LEU:HD21	1:B:282:ILE:HD11	2.00	0.43
1:B:176:PHE:HZ	1:B:402:TYR:HD1	1.67	0.42
1:B:319:ASN:HD21	1:B:321:GLN:HB3	1.84	0.42
1:A:160:SER:OG	1:A:212:SER:HB3	2.18	0.42
1:A:44[A]:THR:CG2	1:A:45[A]:GLY:N	2.83	0.42
1:A:202:THR:O	1:A:203:VAL:HG12	2.14	0.42
1:B:163:PHE:CD2	1:B:166:PHE:CZ	3.00	0.42
1:B:205:ASP:C	1:B:395:ARG:NH1	2.74	0.42
1:B:299:LEU:HD11	1:B:303:LYS:HE2	2.01	0.42
1:A:40[A]:SER:HA	1:A:41[A]:GLY:HA3	1.64	0.42
1:A:157:ALA:HB1	1:A:160:SER:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ARG:HB2	1:A:397:ASP:OD1	2.19	0.42
1:B:150:ILE:HG22	1:B:187:TYR:HD1	1.84	0.42
1:B:190:LEU:HG	1:B:194:ILE:CD1	2.49	0.42
1:A:206:GLU:CA	1:A:398:ARG:HE	2.22	0.42
1:B:52:LEU:HD23	1:B:68:ALA:HA	2.00	0.42
1:A:44[A]:THR:HG22	1:A:45[A]:GLY:N	2.34	0.42
1:A:353:GLN:O	1:A:357:ARG:HG2	2.20	0.42
1:A:44[B]:THR:HG1	1:A:45[B]:GLY:H	1.66	0.42
1:A:162:ASP:C	1:A:163:PHE:O	2.63	0.41
1:A:254:LYS:HD3	1:A:254:LYS:HA	1.36	0.41
1:A:357:ARG:O	1:A:358:SER:CB	2.68	0.41
1:B:52:LEU:HD23	1:B:68:ALA:CA	2.49	0.41
1:B:117:LEU:HD22	1:B:375:THR:HG21	2.03	0.41
1:B:342:ILE:HD13	1:B:347:GLU:C	2.44	0.41
1:A:190:LEU:HG	1:A:194:ILE:HD12	2.02	0.41
1:B:161:THR:O	1:B:162:ASP:C	2.63	0.41
1:B:146:PRO:HD2	1:B:170:PRO:HD2	2.02	0.41
1:A:301:ARG:HD3	1:A:330:LYS:O	2.20	0.41
1:B:338:LYS:HD2	1:B:341:GLN:OE1	2.20	0.41
1:A:40[B]:SER:O	1:A:367:ARG:HB3	2.21	0.40
1:A:193:VAL:O	1:A:197:ARG:HG2	2.22	0.40
1:A:163:PHE:CE1	1:A:273:TRP:HH2	2.39	0.40
1:A:244:PRO:HD2	1:A:286:GLU:O	2.20	0.40
1:A:289:LEU:HD13	1:A:296:GLY:C	2.47	0.40

There are no symmetry-related clashes.

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	427/426 (100%)	383 (90%)	30 (7%)	14 (3%)	3 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	415/426 (97%)	379 (91%)	29 (7%)	7 (2%)	7	12
All	All	842/852 (99%)	762 (90%)	59 (7%)	21 (2%)	5	6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	163	PHE
1	B	264	LEU
1	A	45[A]	GLY
1	A	45[B]	GLY
1	A	46[A]	ALA
1	A	46[B]	ALA
1	A	203	VAL
1	A	255	TYR
1	B	40	SER
1	A	44[A]	THR
1	A	44[B]	THR
1	A	156	HIS
1	A	358	SER
1	B	157	ALA
1	B	155	GLN
1	B	163	PHE
1	A	161	THR
1	B	39	PRO
1	A	214	PRO
1	B	214	PRO

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	333/332 (100%)	321 (96%)	12 (4%)	31	55
1	B	326/332 (98%)	317 (97%)	9 (3%)	38	64
All	All	659/664 (99%)	638 (97%)	21 (3%)	34	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	138	VAL
1	A	143	LEU
1	A	156	HIS
1	A	159	ASN
1	A	194	ILE
1	A	200	SER
1	A	206	GLU
1	A	213	LEU
1	A	254	LYS
1	A	277	VAL
1	A	426	VAL
1	B	4	LEU
1	B	43	SER
1	B	78	GLU
1	B	156	HIS
1	B	160	SER
1	B	197	ARG
1	B	201	THR
1	B	202	THR
1	B	249	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	149	ASN
1	A	152	ASN
1	A	195	HIS
1	A	256	HIS
1	A	341	GLN
1	A	387	GLN
1	B	47	HIS
1	B	88	GLN
1	B	319	ASN
1	B	324	GLN
1	B	341	GLN
1	B	366	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	2PG	B	502[B]	2	9,10,10	1.02	0	12,14,14	1.26	2 (16%)
3	2PG	A	502[B]	-	9,10,10	1.00	0	12,14,14	1.10	1 (8%)

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	2PG	B	502[B]	2	-	2/11/11/11	-
3	2PG	A	502[B]	-	-	3/11/11/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[B]	2PG	O2-C1-C2	2.75	119.87	112.71
3	B	502[B]	2PG	O1-C1-C2	-2.16	118.18	122.85
3	A	502[B]	2PG	O2-C1-C2	2.14	118.26	112.71

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[B]	2PG	C1-C2-C3-O3
3	A	502[B]	2PG	O1P-C2-C3-O3
3	B	502[B]	2PG	C1-C2-C3-O3
3	B	502[B]	2PG	O1P-C2-C3-O3
3	A	502[B]	2PG	C2-O1P-P-O2P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502[B]	2PG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	262:ARG	C	263:SER	N	1.12
1	B	155:GLN	C	156:HIS	N	1.10
1	B	158:THR	C	159:ASN	N	1.04

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	424/426 (99%)	0.89	69 (16%) 4 3	24, 48, 97, 120	7 (1%)
1	B	419/426 (98%)	1.35	110 (26%) 1 1	27, 58, 128, 144	0
All	All	843/852 (98%)	1.12	179 (21%) 2 2	24, 52, 111, 144	7 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44[A]	THR	23.6
1	A	45[A]	GLY	12.2
1	B	42	ALA	9.9
1	A	42[A]	ALA	9.1
1	A	202	THR	8.5
1	A	252	ASP	8.2
1	A	43[A]	SER	8.1
1	B	44	THR	7.2
1	B	426	VAL	7.2
1	A	41[A]	GLY	7.0
1	A	46[A]	ALA	6.9
1	B	45	GLY	6.7
1	B	151	MET	6.7
1	A	203	VAL	6.7
1	B	154	GLY	6.6
1	B	201	THR	6.5
1	B	43	SER	6.4
1	B	202	THR	6.4
1	B	159	ASN	6.3
1	A	426	VAL	6.2
1	B	47	HIS	6.0
1	B	160	SER	6.0
1	B	203	VAL	6.0
1	A	159	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	200	SER	5.9
1	A	205	ASP	5.7
1	B	249	ILE	5.6
1	B	194	ILE	5.6
1	B	158	THR	5.6
1	A	201	THR	5.5
1	B	264	LEU	5.4
1	B	205	ASP	5.3
1	B	209	PHE	5.2
1	A	200	SER	5.1
1	B	199	PHE	5.1
1	A	161	THR	5.1
1	A	264	LEU	5.1
1	B	156	HIS	5.0
1	B	40	SER	5.0
1	A	162	ASP	5.0
1	A	199	PHE	4.9
1	A	40[A]	SER	4.8
1	B	257	LEU	4.8
1	B	210	ALA	4.8
1	B	150	ILE	4.7
1	B	46	ALA	4.7
1	B	213	LEU	4.6
1	B	204	GLY	4.5
1	B	394	ALA	4.5
1	A	194	ILE	4.5
1	A	158	THR	4.5
1	B	206	GLU	4.4
1	B	192	LYS	4.4
1	B	48	GLU	4.3
1	B	218	ALA	4.3
1	B	207	GLY	4.3
1	B	152	ASN	4.2
1	A	207	GLY	4.2
1	B	398	ARG	4.1
1	B	215	THR	4.1
1	B	256	HIS	4.1
1	B	41	GLY	4.0
1	B	223	ILE	4.0
1	B	270	VAL	4.0
1	B	198	GLY	3.9
1	B	211	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	214	PRO	3.9
1	B	190	LEU	3.9
1	B	263	SER	3.9
1	A	157	ALA	3.8
1	B	163	PHE	3.8
1	B	304	LEU	3.8
1	A	247	THR	3.7
1	A	209	PHE	3.7
1	B	193	VAL	3.6
1	B	212	SER	3.6
1	B	208	GLY	3.6
1	B	220	LEU	3.6
1	A	395	ARG	3.6
1	A	191	LYS	3.5
1	B	49	ALA	3.5
1	B	280	TYR	3.5
1	B	222	LEU	3.4
1	A	160	SER	3.4
1	B	258	LYS	3.4
1	A	163	PHE	3.3
1	A	394	ALA	3.3
1	B	247	THR	3.3
1	B	274	VAL	3.3
1	B	273	TRP	3.3
1	B	196	ASP	3.2
1	B	161	THR	3.2
1	B	269	MET	3.2
1	A	265	SER	3.2
1	A	195	HIS	3.2
1	A	261	GLY	3.2
1	B	245	ALA	3.2
1	A	250	PHE	3.2
1	A	47	HIS	3.2
1	B	191	LYS	3.2
1	B	155	GLN	3.2
1	B	197	ARG	3.1
1	B	367	ARG	3.1
1	B	276	LEU	3.1
1	B	153	GLY	3.1
1	B	261	GLY	3.1
1	B	227	ILE	3.1
1	B	303	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	210	ALA	3.0
1	B	195	HIS	3.0
1	A	204	GLY	3.0
1	B	226	ALA	3.0
1	B	216	ASN	3.0
1	A	255	TYR	3.0
1	B	262	ARG	2.9
1	B	277	VAL	2.9
1	B	272	TYR	2.9
1	B	328	GLU	2.9
1	B	425	LYS	2.9
1	A	398	ARG	2.8
1	B	53	ARG	2.8
1	A	197	ARG	2.8
1	A	156	HIS	2.7
1	B	324	GLN	2.7
1	B	282	ILE	2.7
1	B	266	SER	2.7
1	B	52	LEU	2.7
1	A	206	GLU	2.7
1	B	312	GLY	2.7
1	B	300	LEU	2.7
1	A	257	LEU	2.6
1	A	266	SER	2.6
1	A	358	SER	2.6
1	A	214	PRO	2.6
1	A	246	THR	2.6
1	B	246	THR	2.6
1	A	155	GLN	2.6
1	A	258	LYS	2.5
1	B	225	GLU	2.5
1	B	166	PHE	2.5
1	A	425	LYS	2.5
1	B	50	LEU	2.5
1	B	217	ASP	2.4
1	B	157	ALA	2.4
1	B	271	ASP	2.4
1	A	263	SER	2.4
1	A	303	LYS	2.4
1	A	196	ASP	2.4
1	B	341	GLN	2.4
1	A	259	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	296	GLY	2.3
1	A	220	LEU	2.3
1	B	302	ALA	2.3
1	A	253	GLY	2.3
1	B	238	ILE	2.3
1	B	162	ASP	2.3
1	A	302	ALA	2.3
1	B	267	ALA	2.2
1	A	215	THR	2.2
1	A	151	MET	2.2
1	B	289	LEU	2.2
1	A	39	PRO	2.2
1	A	193	VAL	2.2
1	B	299	LEU	2.2
1	A	262	ARG	2.2
1	B	297	TRP	2.2
1	A	188	HIS	2.1
1	B	259	ARG	2.1
1	A	315	PHE	2.1
1	B	164	GLN	2.1
1	A	213	LEU	2.1
1	B	327	ILE	2.1
1	A	270	VAL	2.1
1	A	17	ARG	2.1
1	B	219	PRO	2.1
1	B	275	ASP	2.1
1	A	390	THR	2.0
1	A	192	LYS	2.0
1	B	314	ASP	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 ⓘ

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	2PG	A	502[B]	11/11	0.59	0.32	93,95,100,100	11
3	2PG	B	502[B]	11/11	0.78	0.24	97,99,104,104	11
2	MG	A	501	1/1	0.90	0.18	41,41,41,41	0
2	MG	B	501	1/1	0.94	0.20	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.