



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:11 AM UTC

PDB ID : 6U2T / pdb_00006u2t
Title : Crystal structure of the T-state of maize C4-phosphoenolpyruvate carboxylase in complex with malate
Authors : Carrizosa-Carbajal, E.I.; Munoz-Clares, R.A.; Gonzalez-Segura, L.
Deposited on : 2019-08-20
Resolution : 2.80 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

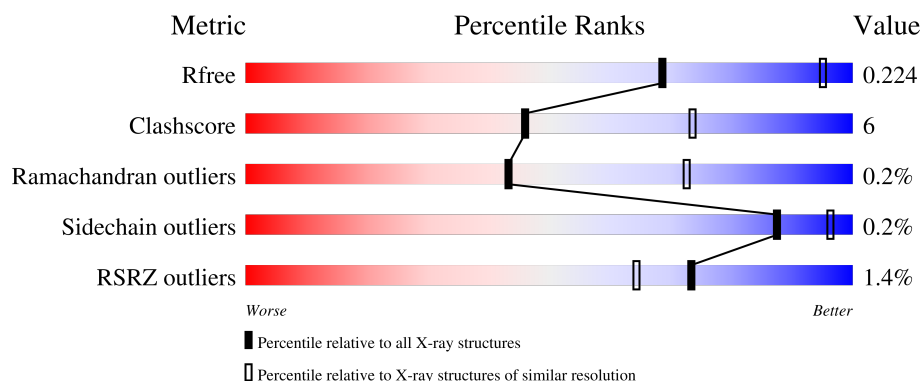
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

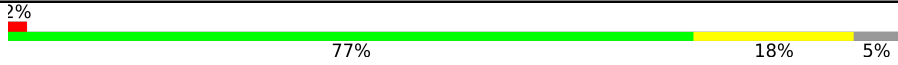
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	970	
1	B	970	
1	C	970	
1	D	970	

2 Entry composition [i](#)

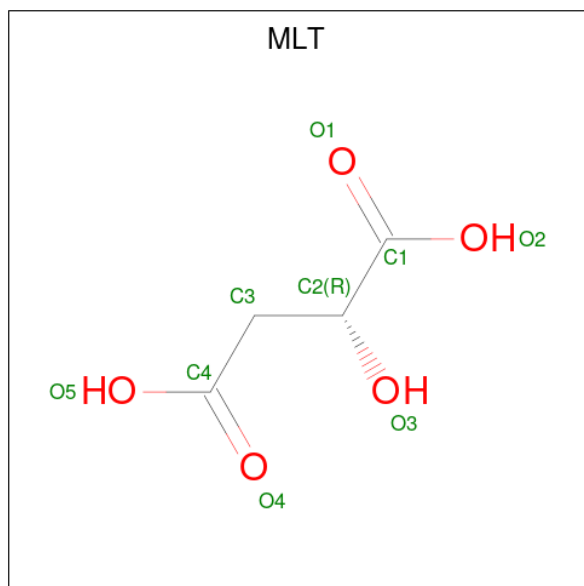
There are 5 unique types of molecules in this entry. The entry contains 29386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	919	Total	C	N	O	S	0	0	0
			7305	4630	1276	1369	30			
1	B	915	Total	C	N	O	S	0	3	0
			7296	4624	1274	1368	30			
1	C	918	Total	C	N	O	S	0	0	0
			7297	4625	1276	1366	30			
1	D	919	Total	C	N	O	S	0	3	0
			7334	4646	1282	1376	30			

- Molecule 2 is D-MALATE (CCD ID: MLT) (formula: C₄H₆O₅).



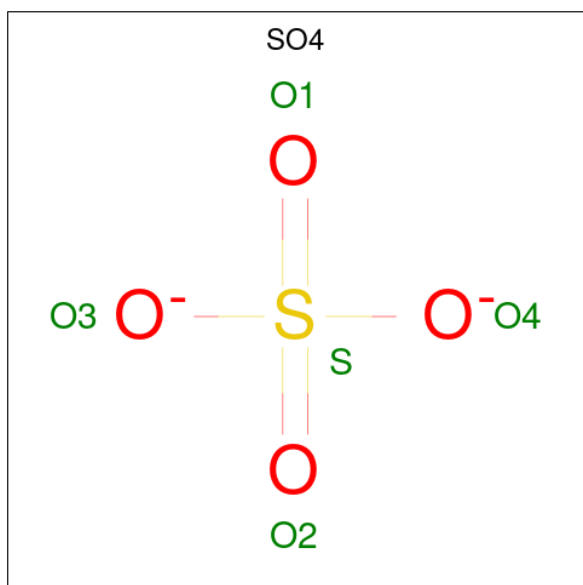
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



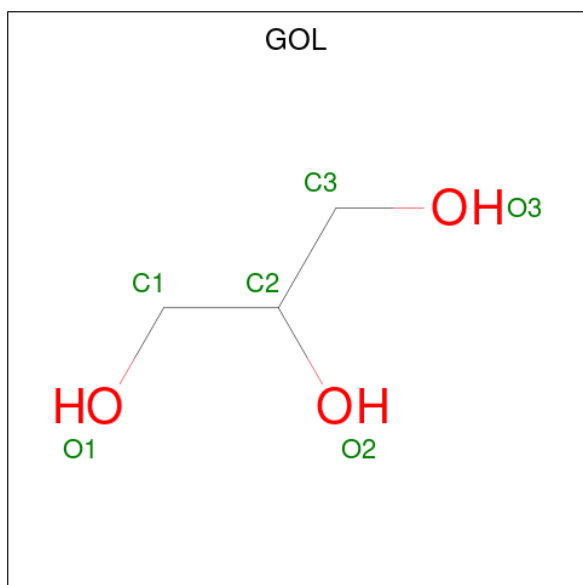
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

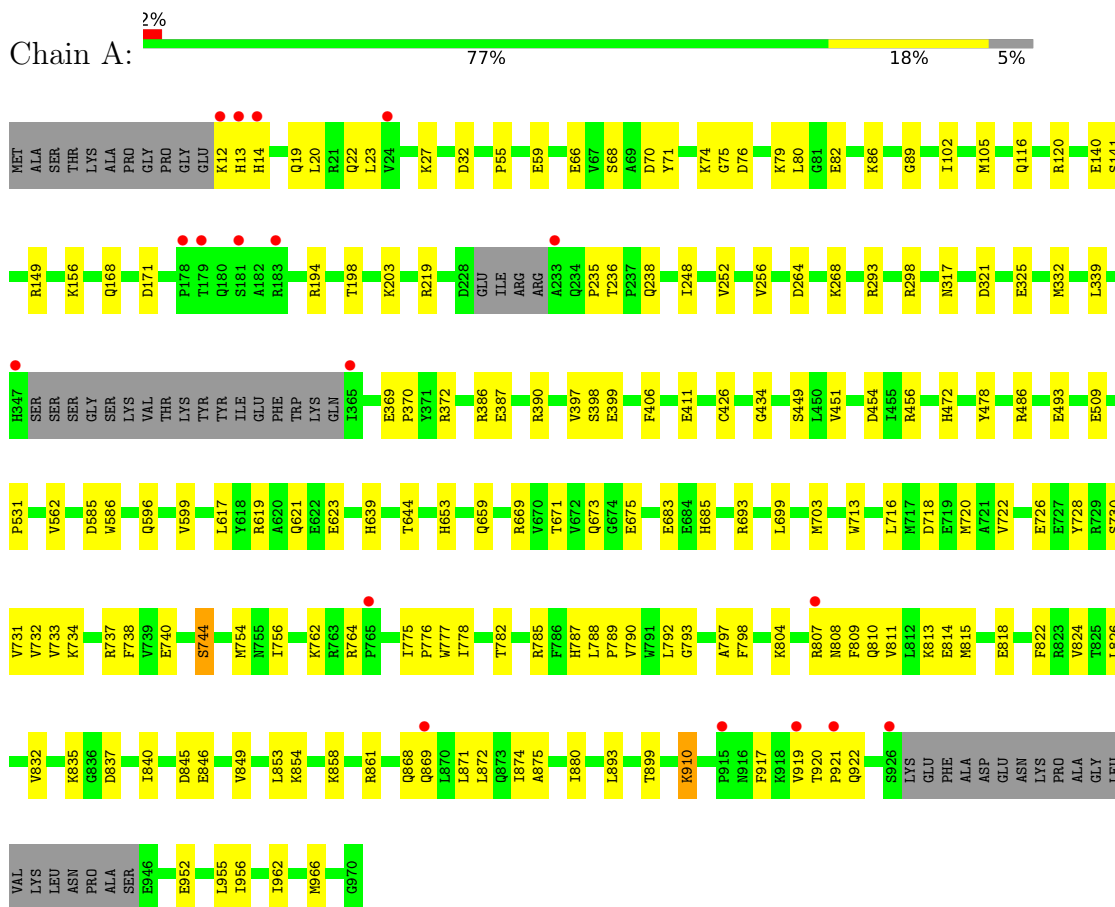
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	12	Total	O	0	0
			12	12		
5	C	21	Total	O	0	0
			21	21		
5	D	21	Total	O	0	0
			21	21		

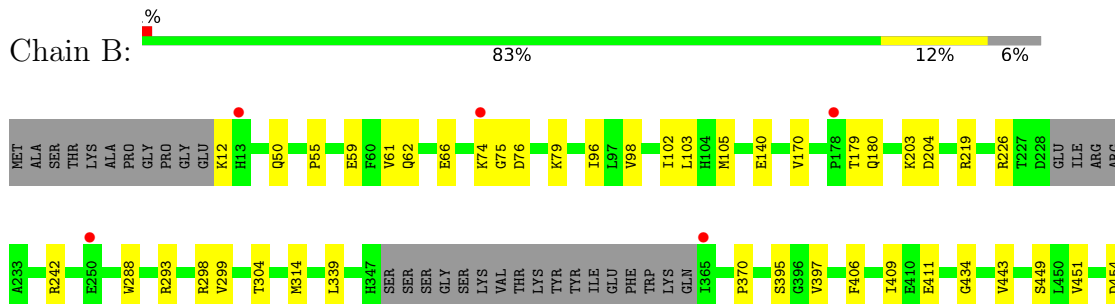
3 Residue-property plots

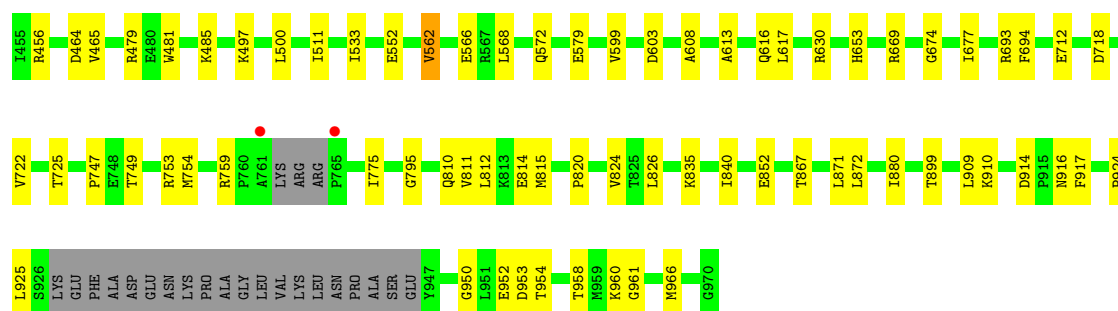
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphoenolpyruvate carboxylase

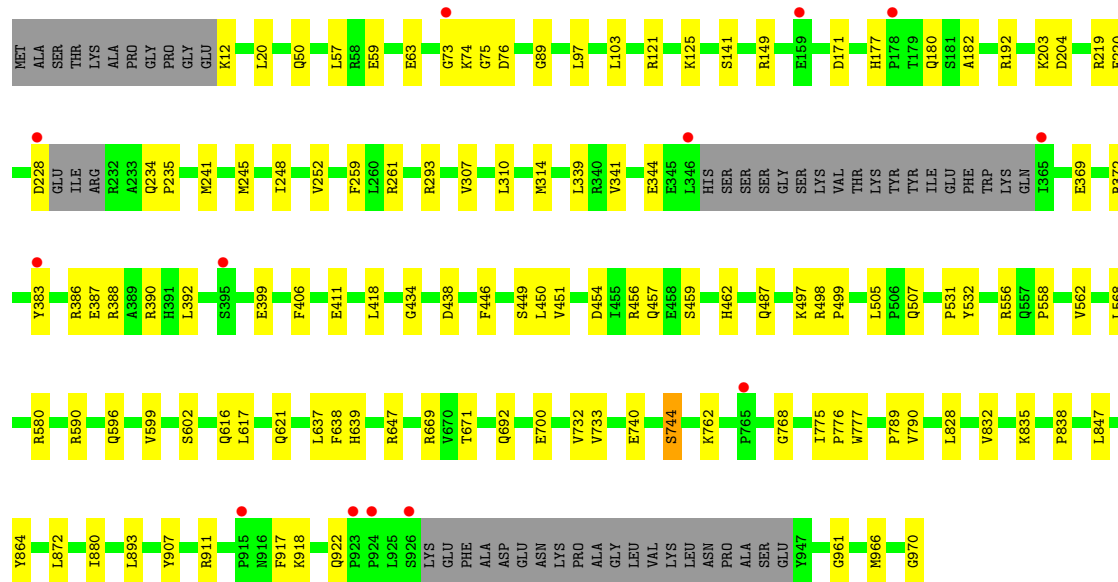
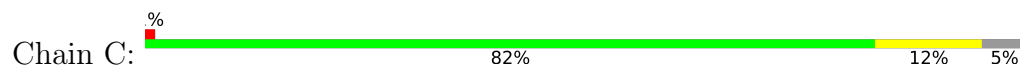


• Molecule 1: Phosphoenolpyruvate carboxylase

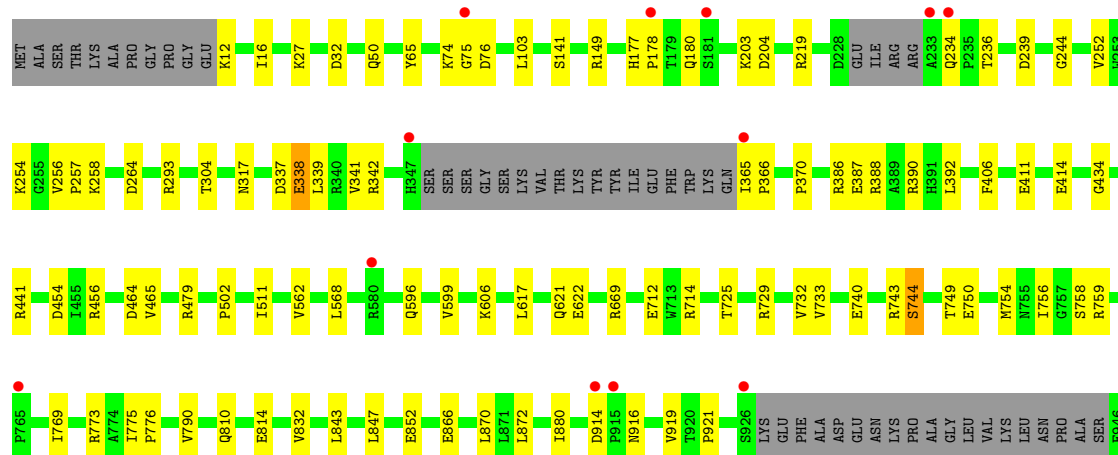
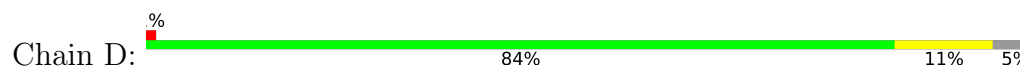




• Molecule 1: Phosphoenolpyruvate carboxylase



• Molecule 1: Phosphoenolpyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.94Å 140.93Å 376.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.80 48.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (48.36-2.80) 94.5 (48.36-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.183 , 0.226 0.185 , 0.224	Depositor DCC
R_{free} test set	6538 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29386	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, MLT

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	0.19	0/7456	0.42	1/10094 (0.0%)
1	B	0.16	0/7446	0.39	0/10079
1	C	0.16	0/7447	0.39	0/10081
1	D	0.16	0/7485	0.38	0/10132
All	All	0.17	0/29834	0.39	1/40386 (0.0%)

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	LYS	CD-CE-NZ	-5.63	93.89	111.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	298	ARG	Peptide
1	D	244	GLY	Peptide

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	7305	0	7299	130	0
1	B	7296	0	7283	72	0
1	C	7297	0	7299	81	0
1	D	7334	0	7321	70	0
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
3	A	10	0	0	1	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	1	0
4	D	6	0	8	0	0
5	A	3	0	0	0	0
5	B	12	0	0	0	0
5	C	21	0	0	0	0
5	D	21	0	0	0	0
All	All	29386	0	29226	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 6.

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:D:759:ARG:HH22	1:D:775:ILE:HD13	1.25	0.97
1:A:754:MET:HE1	1:A:955:LEU:HD23	1.58	0.85
1:A:910:LYS:NZ	1:A:917:PHE:CD2	2.50	0.80
1:C:89:GLY:HA3	1:C:922:GLN:HE21	1.48	0.79
1:C:203:LYS:HD3	1:C:204:ASP:H	1.50	0.76
1:A:910:LYS:NZ	1:A:917:PHE:CG	2.53	0.76
1:A:788:LEU:HD11	1:A:792:LEU:HD12	1.67	0.76
1:B:465:VAL:HG22	1:B:511:ILE:HG23	1.70	0.74
1:A:79:LYS:HA	1:A:82:GLU:HG3	1.71	0.73
1:C:599:VAL:HB	1:C:617:LEU:HD11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:HD21	1:C:97:LEU:HD23	1.71	0.73
1:D:622:GLU:OE2	1:D:714:ARG:NH2	2.23	0.71
1:D:464:ASP:OD1	1:D:479:ARG:NH1	2.25	0.70
1:B:568:LEU:O	1:B:572:GLN:HG3	1.92	0.70
1:B:759:ARG:HH22	1:B:775:ILE:HD13	1.56	0.70
1:D:775:ILE:H	1:D:775:ILE:HD12	1.57	0.70
1:B:464:ASP:OD1	1:B:479:ARG:NH1	2.21	0.69
1:B:835:LYS:HB3	1:B:966:MET:HE1	1.73	0.69
1:D:12:LYS:HG3	1:D:50:GLN:HE22	1.57	0.69
1:D:254:LYS:O	1:D:258:LYS:HD3	1.91	0.69
1:B:76:ASP:HB3	1:B:79:LYS:HE2	1.75	0.68
1:D:759:ARG:NH2	1:D:775:ILE:HD13	2.05	0.68
1:A:754:MET:HE2	1:A:952:GLU:HG3	1.76	0.67
1:C:245:MET:HG3	1:C:314:MET:HE1	1.77	0.66
1:A:756:ILE:HD11	1:A:956:ILE:HD12	1.78	0.66
1:A:762:LYS:HG2	1:A:764:ARG:O	1.96	0.66
1:D:810:GLN:O	1:D:814:GLU:HG3	1.97	0.65
1:A:55:PRO:O	1:A:59:GLU:HG3	1.97	0.65
1:A:798:PHE:HZ	1:A:826:LEU:HD11	1.60	0.65
1:D:754:MET:HE2	1:D:952:GLU:HG3	1.78	0.65
1:A:730:SER:HA	1:A:734:LYS:HG2	1.79	0.65
1:A:456:ARG:NH2	3:A:1002:SO4:O3	2.30	0.64
1:A:835:LYS:HB3	1:A:966:MET:HE1	1.79	0.64
1:B:872:LEU:HD21	1:B:880:ILE:HD13	1.79	0.64
1:A:20:LEU:HD22	1:A:893:LEU:HD22	1.78	0.64
1:A:778:ILE:O	1:A:782:THR:HG23	1.98	0.64
1:B:811:VAL:HG12	1:B:815:MET:HE2	1.77	0.64
1:A:621:GLN:HE22	1:A:659:GLN:HE21	1.45	0.64
1:A:726:GLU:O	1:A:730:SER:OG	2.16	0.63
1:B:203:LYS:HE3	1:B:204:ASP:H	1.64	0.63
1:D:454:ASP:OD2	1:D:669:ARG:NH2	2.27	0.63
1:A:102:ILE:HA	1:A:105:MET:HE3	1.78	0.63
1:C:241:MET:HE3	1:C:307:VAL:HB	1.80	0.63
1:D:750:GLU:O	1:D:754:MET:HG3	1.97	0.63
1:A:728:TYR:HA	1:A:792:LEU:HD22	1.81	0.63
1:A:399:GLU:N	1:C:399:GLU:OE2	2.27	0.63
1:A:807:ARG:NH1	1:A:807:ARG:HA	2.14	0.63
1:B:812:LEU:HA	1:B:815:MET:HE3	1.79	0.62
1:C:203:LYS:HD3	1:C:204:ASP:N	2.14	0.62
1:D:725:THR:O	1:D:729:ARG:HG3	1.99	0.62
1:B:96:ILE:HD11	1:B:953:ASP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:SER:HA	1:C:399:GLU:OE2	2.00	0.62
1:A:744:SER:HB2	1:A:849:VAL:HG12	1.82	0.62
1:B:406:PHE:HD1	1:B:411:GLU:HG3	1.65	0.62
1:C:59:GLU:O	1:C:63:GLU:HG3	2.00	0.61
1:A:869:GLN:N	1:A:869:GLN:OE1	2.34	0.61
1:B:599:VAL:HB	1:B:617:LEU:HD11	1.82	0.61
1:B:795:GLY:HA3	1:B:867:THR:HG22	1.82	0.61
1:A:872:LEU:HD21	1:A:880:ILE:HD13	1.83	0.60
1:A:809:PHE:CZ	1:A:813:LYS:HD3	2.35	0.60
1:A:621:GLN:HE22	1:A:659:GLN:NE2	1.98	0.60
1:B:74:LYS:O	1:B:79:LYS:HE3	2.02	0.60
1:D:338[A]:GLU:OE2	1:D:338[A]:GLU:N	2.28	0.60
1:C:639:HIS:O	1:C:671:THR:HG23	2.02	0.59
1:A:599:VAL:HB	1:A:617:LEU:HD11	1.84	0.59
1:C:241:MET:HG2	1:C:307:VAL:HG12	1.84	0.59
1:B:754:MET:HE2	1:B:952:GLU:HG3	1.85	0.59
1:A:785:ARG:HH12	1:A:899:THR:HG22	1.68	0.59
1:A:639:HIS:O	1:A:671:THR:HG23	2.04	0.58
1:A:194:ARG:O	1:A:198:THR:HG23	2.04	0.58
1:A:910:LYS:NZ	1:A:917:PHE:CE2	2.70	0.58
1:C:57:LEU:HD12	1:C:57:LEU:O	2.04	0.58
1:D:775:ILE:HD12	1:D:775:ILE:N	2.19	0.58
1:A:86:LYS:O	1:A:922:GLN:NE2	2.36	0.57
1:D:236:THR:HG23	1:D:239:ASP:H	1.69	0.57
1:D:406:PHE:HD1	1:D:411:GLU:HG3	1.70	0.57
1:A:910:LYS:NZ	1:A:917:PHE:CD1	2.71	0.57
1:C:462:HIS:HE1	1:C:532:TYR:OH	1.87	0.57
1:A:790:VAL:HG11	1:A:832:VAL:HG21	1.86	0.57
1:A:493:GLU:OE1	1:C:498:ARG:NH2	2.36	0.56
1:C:341:VAL:O	1:C:344:GLU:HG2	2.06	0.56
1:D:317:ASN:OD1	1:D:386:ARG:NH1	2.35	0.56
1:D:617:LEU:O	1:D:621:GLN:HG3	2.06	0.56
1:C:835:LYS:HB3	1:C:966:MET:HE1	1.88	0.56
1:D:562:VAL:HG22	1:D:596:GLN:HB3	1.88	0.56
1:A:171:ASP:HB3	1:A:669:ARG:HG2	1.86	0.56
1:A:814:GLU:HG2	1:A:818:GLU:OE1	2.06	0.56
1:B:914:ASP:OD2	1:B:916:ASN:N	2.34	0.55
1:C:498:ARG:HG2	1:C:499:PRO:HD2	1.88	0.55
1:A:236:THR:HG22	1:A:238:GLN:H	1.70	0.55
1:B:180:GLN:HG2	1:B:960:LYS:HE2	1.89	0.55
1:C:57:LEU:CD2	1:C:97:LEU:HD23	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:SER:OG	1:A:149:ARG:NH2	2.39	0.55
1:D:465:VAL:HG22	1:D:511:ILE:HG23	1.88	0.55
1:A:406:PHE:HD1	1:A:411:GLU:HG3	1.71	0.55
1:A:798:PHE:CZ	1:A:826:LEU:HD11	2.41	0.55
1:C:647:ARG:HD2	1:C:828:LEU:HD23	1.88	0.55
1:A:252:VAL:O	1:A:256:VAL:HG23	2.06	0.55
1:A:952:GLU:O	1:A:956:ILE:HG12	2.05	0.55
1:C:12:LYS:HG3	1:C:50:GLN:HE22	1.72	0.54
1:A:849:VAL:HG23	1:A:854:LYS:HG2	1.89	0.54
1:B:449:SER:O	1:B:451:VAL:N	2.40	0.54
1:C:73:GLY:C	1:C:74:LYS:HD2	2.33	0.54
1:A:12:LYS:HG3	1:A:13:HIS:CE1	2.43	0.54
1:A:737:ARG:HH21	1:A:853:LEU:HD11	1.72	0.54
1:A:236:THR:HG22	1:A:238:GLN:OE1	2.07	0.54
1:B:810:GLN:O	1:B:814:GLU:HG3	2.08	0.53
1:A:168:GLN:HE22	1:A:699:LEU:HA	1.74	0.53
1:C:790:VAL:HG11	1:C:832:VAL:HG21	1.89	0.53
1:D:387:GLU:OE2	1:D:390:ARG:NH1	2.42	0.53
1:A:156:LYS:HE3	1:A:703:MET:HB3	1.91	0.53
1:D:177:HIS:HD2	1:D:178:PRO:HD2	1.74	0.53
1:A:397:VAL:HG13	1:C:399:GLU:HG3	1.91	0.53
1:C:459:SER:HA	1:C:462:HIS:HD2	1.73	0.53
1:C:556:ARG:H	1:C:556:ARG:HD2	1.73	0.53
1:A:219:ARG:HD3	1:B:434:GLY:HA3	1.91	0.53
1:A:720:MET:HB3	1:A:797:ALA:HB1	1.91	0.53
1:A:754:MET:HE2	1:A:952:GLU:CG	2.39	0.53
1:D:622:GLU:CD	1:D:714:ARG:HH22	2.17	0.53
1:A:70:ASP:HB3	1:A:74:LYS:HE2	1.91	0.52
1:A:814:GLU:O	1:A:818:GLU:HG3	2.09	0.52
1:B:454:ASP:OD2	1:B:669:ARG:NH2	2.35	0.52
1:A:12:LYS:HG3	1:A:13:HIS:ND1	2.24	0.52
1:A:962:ILE:O	1:A:966:MET:HG2	2.09	0.52
1:B:179:THR:O	1:B:960:LYS:HE3	2.09	0.52
1:D:234:GLN:CD	1:D:758:SER:OG	2.52	0.52
1:B:500:LEU:HB3	1:B:552:GLU:HG3	1.92	0.52
1:D:293:ARG:NH2	1:D:304:THR:OG1	2.37	0.52
1:D:365:ILE:HG23	1:D:366:PRO:HD3	1.90	0.52
1:A:845:ASP:O	1:A:849:VAL:HG22	2.10	0.51
1:C:203:LYS:HE2	1:C:203:LYS:HA	1.93	0.51
1:A:19:GLN:O	1:A:23:LEU:HD13	2.10	0.51
1:A:434:GLY:HA3	1:B:219:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:HA	1:A:509:GLU:OE1	2.09	0.51
1:B:242:ARG:HD3	1:B:314:MET:HE2	1.91	0.51
1:D:790:VAL:HG11	1:D:832:VAL:HG21	1.93	0.51
1:C:487:GLN:OE1	1:C:580:ARG:NE	2.43	0.51
1:C:121:ARG:HH22	1:C:125:LYS:HZ1	1.57	0.51
1:A:562:VAL:HG22	1:A:596:GLN:HB3	1.93	0.51
1:A:619:ARG:O	1:A:623:GLU:HG3	2.10	0.51
1:D:254:LYS:O	1:D:258:LYS:CD	2.59	0.51
1:A:731:VAL:HG12	1:A:738:PHE:CE1	2.46	0.51
1:A:920:THR:O	1:A:920:THR:OG1	2.29	0.51
1:B:96:ILE:HD13	1:B:954:THR:HG22	1.93	0.51
1:B:795:GLY:CA	1:B:867:THR:HG22	2.41	0.51
1:D:339:LEU:HD21	1:D:370:PRO:HB2	1.93	0.51
1:C:369:GLU:HB3	1:C:372:ARG:HD2	1.93	0.50
1:D:252:VAL:O	1:D:256:VAL:HG23	2.11	0.50
1:A:317:ASN:OD1	1:A:386:ARG:NH1	2.38	0.50
1:C:20:LEU:HD22	1:C:893:LEU:HD22	1.93	0.50
1:C:406:PHE:HD1	1:C:411:GLU:HG3	1.76	0.50
1:A:737:ARG:NH2	1:A:853:LEU:HD11	2.27	0.50
1:C:562:VAL:HG22	1:C:596:GLN:HB3	1.93	0.50
1:B:55:PRO:O	1:B:59:GLU:HG3	2.12	0.50
1:C:775:ILE:HB	1:C:776:PRO:HD3	1.93	0.50
1:D:342:ARG:HH12	1:D:414:GLU:CD	2.18	0.50
1:A:809:PHE:CE2	1:A:813:LYS:HD3	2.47	0.50
1:A:807:ARG:O	1:A:807:ARG:HD3	2.11	0.49
1:B:749:THR:O	1:B:753:ARG:HG3	2.12	0.49
1:D:740:GLU:O	1:D:744:SER:OG	2.30	0.49
1:A:369:GLU:OE2	1:A:372:ARG:HD2	2.12	0.49
1:D:141:SER:OG	1:D:149:ARG:NH2	2.44	0.49
1:C:732:VAL:HG23	1:C:733:VAL:HG23	1.93	0.49
1:D:177:HIS:CE1	1:D:180:GLN:HB3	2.47	0.49
1:A:826:LEU:HD12	1:A:871:LEU:HD13	1.94	0.49
1:B:566:GLU:HB3	1:B:603:ASP:HB3	1.94	0.49
1:C:558:PRO:HD2	1:C:590:ARG:NH2	2.28	0.49
1:A:339:LEU:CD2	1:A:370:PRO:HB2	2.43	0.49
1:A:339:LEU:HD21	1:A:370:PRO:HB2	1.95	0.49
1:A:449:SER:O	1:A:451:VAL:N	2.43	0.49
1:D:12:LYS:HG3	1:D:50:GLN:NE2	2.27	0.49
1:D:12:LYS:HG2	1:D:12:LYS:O	2.13	0.49
1:D:203:LYS:NZ	1:D:204:ASP:OD2	2.45	0.49
1:A:454:ASP:OD1	1:A:531:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ARG:NH1	1:C:700:GLU:OE1	2.45	0.49
1:A:874:ILE:O	1:A:875:ALA:HB3	2.13	0.48
1:B:74:LYS:O	1:B:76:ASP:N	2.46	0.48
1:B:568:LEU:HD21	1:B:613:ALA:HA	1.94	0.48
1:B:339:LEU:HD21	1:B:370:PRO:HB2	1.95	0.48
1:A:822:PHE:O	1:A:826:LEU:HD23	2.14	0.48
1:C:141:SER:OG	1:C:149:ARG:NH2	2.46	0.48
1:A:868:GLN:HB3	1:A:869:GLN:OE1	2.13	0.48
1:A:835:LYS:HB3	1:A:966:MET:CE	2.44	0.48
1:C:177:HIS:CD2	1:C:180:GLN:HB3	2.49	0.48
1:C:293:ARG:HG2	1:C:456:ARG:O	2.13	0.48
1:C:740:GLU:O	1:C:744:SER:OG	2.31	0.47
1:D:743:ARG:HH21	1:D:749:THR:HG22	1.79	0.47
1:A:19:GLN:O	1:A:22:GLN:HG2	2.14	0.47
1:A:807:ARG:HA	1:A:807:ARG:CZ	2.43	0.47
1:A:919:VAL:O	1:A:921:PRO:HD3	2.14	0.47
1:B:12:LYS:HD3	1:B:50:GLN:NE2	2.29	0.47
1:C:180:GLN:HE22	1:C:182:ALA:HA	1.79	0.47
1:C:339:LEU:HD12	1:C:418:LEU:HG	1.96	0.47
1:D:103:LEU:HD13	1:D:961:GLY:HA2	1.96	0.47
1:A:140:GLU:OE2	1:A:693:ARG:NH1	2.47	0.47
1:A:732:VAL:HG12	1:A:733:VAL:HG23	1.95	0.47
1:D:843:LEU:O	1:D:847:LEU:HD23	2.14	0.47
1:C:621:GLN:HE21	1:C:637:LEU:HD13	1.80	0.47
1:B:96:ILE:CD1	1:B:953:ASP:HB2	2.45	0.47
1:D:919:VAL:O	1:D:921:PRO:HD3	2.14	0.47
1:B:810:GLN:HG3	1:B:814:GLU:OE1	2.15	0.47
1:C:838:PRO:HG3	1:C:864:TYR:CE1	2.49	0.47
1:B:950:GLY:O	1:B:954:THR:HG23	2.14	0.47
1:C:872:LEU:HD21	1:C:880:ILE:HD13	1.96	0.47
1:A:12:LYS:O	1:A:12:LYS:NZ	2.47	0.47
1:C:74:LYS:O	1:C:76:ASP:N	2.47	0.47
1:D:754:MET:HB2	1:D:756:ILE:CD1	2.45	0.47
1:A:293:ARG:HG2	1:A:456:ARG:O	2.15	0.46
1:A:716:LEU:O	1:A:720:MET:HG3	2.15	0.46
1:A:740:GLU:O	1:A:744:SER:OG	2.33	0.46
1:C:171:ASP:HB3	1:C:669:ARG:HG2	1.96	0.46
1:A:713:TRP:CD1	1:A:815:MET:HE2	2.49	0.46
1:A:89:GLY:C	1:A:922:GLN:HE21	2.24	0.46
1:A:321:ASP:O	1:A:325:GLU:HG3	2.15	0.46
1:B:62:GLN:O	1:B:66:GLU:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ARG:NH2	1:B:304:THR:OG1	2.36	0.46
1:B:759:ARG:NH2	1:B:775:ILE:HD13	2.27	0.46
1:B:820:PRO:O	1:B:824:VAL:HG13	2.15	0.46
1:A:846:GLU:HA	1:A:854:LYS:HE2	1.98	0.46
1:D:775:ILE:H	1:D:775:ILE:CD1	2.28	0.46
1:D:872:LEU:HD21	1:D:880:ILE:HD13	1.98	0.46
1:A:32:ASP:HA	1:A:116:GLN:NE2	2.31	0.46
1:A:858:LYS:HE2	1:A:861:ARG:HH21	1.80	0.46
1:D:74:LYS:O	1:D:76:ASP:N	2.48	0.46
1:B:140:GLU:OE2	1:B:693:ARG:NH1	2.49	0.46
1:B:924:PRO:C	1:B:925:LEU:HD12	2.40	0.46
1:B:910:LYS:HE3	1:B:917:PHE:CD1	2.50	0.46
1:C:310:LEU:O	1:C:314:MET:HG3	2.16	0.46
1:D:954:THR:O	1:D:958:THR:HG23	2.15	0.46
1:A:71:TYR:CG	1:A:80:LEU:HD11	2.51	0.45
1:B:409:ILE:HD11	1:B:443:VAL:HG13	1.98	0.45
1:C:568:LEU:HD13	1:C:616:GLN:HG2	1.97	0.45
1:D:339:LEU:CD2	1:D:370:PRO:HB2	2.45	0.45
1:D:866:GLU:O	1:D:870:LEU:HD23	2.16	0.45
1:B:840:ILE:HD11	1:B:899:THR:HG23	1.98	0.45
1:C:261:ARG:NH2	1:C:438:ASP:OD2	2.43	0.45
1:D:256:VAL:HB	1:D:257:PRO:HD3	1.99	0.45
1:C:103:LEU:HD13	1:C:961:GLY:HA2	1.98	0.45
1:D:16:ILE:HB	1:D:65:TYR:CE2	2.52	0.45
1:D:337:ASP:O	1:D:341:VAL:HG23	2.16	0.45
1:A:168:GLN:HE22	1:A:699:LEU:CA	2.30	0.45
1:B:775:ILE:HD12	1:B:775:ILE:H	1.82	0.45
1:C:638:PHE:CE1	1:C:671:THR:HG22	2.51	0.45
1:C:777:TRP:NE1	1:C:789:PRO:HB3	2.32	0.45
1:A:478:TYR:CZ	1:A:486:ARG:HD3	2.51	0.45
1:B:293:ARG:HG2	1:B:456:ARG:O	2.16	0.45
1:B:747:PRO:HB3	1:B:909:LEU:HD11	1.98	0.45
1:D:599:VAL:HB	1:D:617:LEU:HD11	1.98	0.44
1:A:74:LYS:O	1:A:76:ASP:N	2.51	0.44
1:B:103:LEU:HD13	1:B:961:GLY:HA2	1.99	0.44
1:B:339:LEU:CD2	1:B:370:PRO:HB2	2.47	0.44
1:A:718:ASP:O	1:A:722:VAL:HG23	2.16	0.44
1:C:556:ARG:H	1:C:556:ARG:CD	2.30	0.44
1:B:835:LYS:HB3	1:B:966:MET:CE	2.46	0.44
1:C:219:ARG:HD3	1:D:434:GLY:HA3	1.99	0.44
1:C:454:ASP:OD1	1:C:531:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:ARG:O	1:D:392:LEU:HG	2.18	0.44
1:B:954:THR:O	1:B:958:THR:HG23	2.18	0.44
1:A:785:ARG:HH12	1:A:899:THR:CG2	2.30	0.44
1:A:713:TRP:HA	1:A:815:MET:HE2	1.99	0.44
1:A:826:LEU:HD12	1:A:871:LEU:CD1	2.48	0.44
1:A:116:GLN:OE1	1:A:120:ARG:NH2	2.47	0.43
1:C:234:GLN:HG3	1:C:235:PRO:HD2	2.00	0.43
1:A:585:ASP:OD1	1:A:586:TRP:N	2.52	0.43
1:B:608:ALA:HB1	1:B:725:THR:HG23	2.00	0.43
1:C:602:SER:OG	1:C:970:GLY:OXT	2.27	0.43
1:B:572:GLN:HG2	1:B:616:GLN:OE1	2.19	0.43
1:B:718:ASP:O	1:B:722:VAL:HG23	2.19	0.43
1:B:712:GLU:H	1:B:712:GLU:HG3	1.62	0.43
1:C:449:SER:O	1:C:451:VAL:N	2.47	0.43
1:D:293:ARG:HG2	1:D:456:ARG:O	2.19	0.43
1:A:79:LYS:HD3	1:A:82:GLU:CD	2.44	0.43
1:A:792:LEU:HD23	1:A:793:GLY:N	2.33	0.43
1:A:808:ASN:O	1:A:811:VAL:HG12	2.18	0.43
1:C:911:ARG:HG2	1:C:917:PHE:CE2	2.54	0.43
1:C:387:GLU:OE2	1:C:390:ARG:NH1	2.52	0.43
1:C:228:ASP:OD1	1:C:228:ASP:N	2.52	0.43
1:D:775:ILE:HB	1:D:776:PRO:HD3	2.00	0.43
1:A:807:ARG:NH1	1:A:810:GLN:HB3	2.34	0.42
1:C:762:LYS:NZ	1:C:768:GLY:O	2.51	0.42
1:C:847:LEU:HD11	1:C:907:TYR:CE1	2.54	0.42
1:D:732:VAL:HG23	1:D:733:VAL:HG23	2.00	0.42
1:A:837:ASP:OD2	1:A:840:ILE:HG12	2.19	0.42
1:B:102:ILE:HA	1:B:105:MET:HE3	2.01	0.42
1:C:57:LEU:HD21	1:C:97:LEU:CD2	2.46	0.42
1:D:365:ILE:CG2	1:D:366:PRO:HD3	2.49	0.42
1:A:426:CYS:O	1:B:226:ARG:NH2	2.53	0.42
1:B:61:VAL:HG22	1:B:98:VAL:HG13	2.01	0.42
1:B:674:GLY:O	1:B:677:ILE:HG22	2.19	0.42
1:C:388:ARG:O	1:C:392:LEU:HG	2.19	0.42
1:D:914:ASP:OD1	1:D:916:ASN:N	2.41	0.42
1:C:259:PHE:CE1	1:C:692:GLN:HA	2.55	0.42
1:A:653:HIS:HB2	1:A:693:ARG:HG2	2.01	0.42
1:D:264:ASP:CG	1:D:441:ARG:HH22	2.28	0.42
1:A:720:MET:HE1	1:A:798:PHE:CD1	2.55	0.42
1:C:434:GLY:HA3	1:D:219:ARG:HD3	2.00	0.42
1:B:288:TRP:CD1	1:B:454:ASP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:CG2	1:A:238:GLN:OE1	2.68	0.42
1:A:248:ILE:HA	1:A:252:VAL:HB	2.02	0.42
1:C:922:GLN:H	1:C:922:GLN:HG2	1.70	0.42
1:C:248:ILE:HA	1:C:252:VAL:HB	2.02	0.42
1:C:293:ARG:HG3	1:C:457:GLN:NE2	2.35	0.42
1:D:775:ILE:HD11	3:D:1002:SO4:S	2.60	0.42
1:A:683:GLU:OE1	1:A:685:HIS:N	2.51	0.42
1:D:606:LYS:HZ2	1:D:769:ILE:HG23	1.84	0.42
1:A:787:HIS:CE1	1:A:966:MET:HE2	2.55	0.41
1:B:579:GLU:CD	1:B:630:ARG:HH22	2.28	0.41
1:B:653:HIS:HB2	1:B:693:ARG:HG2	2.01	0.41
1:A:777:TRP:NE1	1:A:789:PRO:HB3	2.35	0.41
1:C:121:ARG:HH22	1:C:125:LYS:NZ	2.17	0.41
1:A:804:LYS:HE3	1:A:804:LYS:O	2.21	0.41
1:B:170:VAL:HG11	1:B:694:PHE:HB3	2.01	0.41
1:B:826:LEU:HD23	1:B:871:LEU:HD12	2.03	0.41
1:D:712:GLU:H	1:D:712:GLU:CD	2.29	0.41
1:A:68:SER:HB3	1:A:899:THR:OG1	2.21	0.41
1:A:775:ILE:HB	1:A:776:PRO:HD3	2.03	0.41
1:B:481:TRP:CG	1:B:485:LYS:HD3	2.56	0.41
1:D:254:LYS:HB2	1:D:254:LYS:HE2	1.92	0.41
1:C:192:ARG:HE	1:C:220:GLU:CD	2.28	0.41
1:A:14:HIS:NE2	1:A:66:GLU:OE2	2.53	0.41
1:A:27:LYS:HB3	1:A:32:ASP:HB3	2.02	0.41
1:A:235:PRO:O	1:A:298:ARG:NH2	2.54	0.41
1:A:673:GLN:NE2	1:A:675:GLU:OE2	2.53	0.41
1:B:533:ILE:HG12	1:B:562:VAL:HG22	2.03	0.41
1:C:505:LEU:O	1:C:507:GLN:HG3	2.20	0.41
1:D:27:LYS:HB3	1:D:32:ASP:HB3	2.03	0.41
1:D:773:ARG:HE	1:D:773:ARG:HB3	1.72	0.41
1:A:264:ASP:O	1:A:268:LYS:HG2	2.21	0.41
1:A:472:HIS:CE1	1:C:497:LYS:HD3	2.56	0.41
1:C:259:PHE:CZ	1:C:692:GLN:HA	2.56	0.41
1:D:852:GLU:OE1	1:D:852:GLU:N	2.52	0.41
1:D:969:THR:OG1	1:D:970:GLY:N	2.53	0.41
1:A:617:LEU:O	1:A:621:GLN:HG3	2.21	0.40
1:B:395:SER:OG	1:B:397:VAL:HG12	2.21	0.40
1:C:383:TYR:HD1	1:C:386:ARG:HH21	1.67	0.40
1:B:497:LYS:O	1:D:502:PRO:HB3	2.22	0.40
1:C:446:PHE:HB3	1:C:450:LEU:HA	2.02	0.40
1:C:762:LYS:HE3	1:C:762:LYS:HB3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:918:LYS:HD3	1:C:918:LYS:HA	1.68	0.40
1:A:387:GLU:OE2	1:A:390:ARG:NH1	2.55	0.40
1:A:644:THR:HG21	1:A:824:VAL:HG12	2.03	0.40
1:B:852:GLU:H	1:B:852:GLU:CD	2.29	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	911/970 (94%)	890 (98%)	19 (2%)	2 (0%)	43	72
1	B	908/970 (94%)	882 (97%)	24 (3%)	2 (0%)	43	72
1	C	910/970 (94%)	894 (98%)	15 (2%)	1 (0%)	48	77
1	D	914/970 (94%)	892 (98%)	21 (2%)	1 (0%)	48	77
All	All	3643/3880 (94%)	3558 (98%)	79 (2%)	6 (0%)	43	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	LYS
1	B	299	VAL
1	A	75	GLY
1	B	75	GLY
1	C	75	GLY
1	D	75	GLY

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	790/832 (95%)	788 (100%)	2 (0%)	86	95
1	B	789/832 (95%)	788 (100%)	1 (0%)	88	97
1	C	789/832 (95%)	788 (100%)	1 (0%)	88	97
1	D	793/832 (95%)	789 (100%)	4 (0%)	81	93
All	All	3161/3328 (95%)	3153 (100%)	8 (0%)	87	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	MET
1	A	744	SER
1	B	562	VAL
1	C	744	SER
1	D	338[A]	GLU
1	D	338[B]	GLU
1	D	568	LEU
1	D	744	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	168	GLN
1	A	177	HIS
1	A	273	ASN
1	A	377	HIS
1	A	391	HIS
1	A	472	HIS
1	A	507	GLN
1	A	519	HIS
1	A	621	GLN
1	A	659	GLN
1	A	665	ASN
1	A	889	GLN
1	A	922	GLN
1	A	967	GLN

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Mol	Chain	Res	Type
1	B	19	GLN
1	B	22	GLN
1	B	218	GLN
1	B	322	GLN
1	B	472	HIS
1	B	596	GLN
1	B	665	ASN
1	B	673	GLN
1	B	810	GLN
1	B	817	ASN
1	C	53	HIS
1	C	167	ASN
1	C	188	GLN
1	C	234	GLN
1	C	322	GLN
1	C	377	HIS
1	C	462	HIS
1	C	595	GLN
1	C	621	GLN
1	C	659	GLN
1	C	665	ASN
1	C	673	GLN
1	C	817	ASN
1	C	922	GLN
1	C	967	GLN
1	D	13	HIS
1	D	177	HIS
1	D	273	ASN
1	D	322	GLN
1	D	377	HIS
1	D	519	HIS
1	D	596	GLN
1	D	673	GLN
1	D	755	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	MLT	C	1001	-	8,8,8	1.08	0	10,10,10	1.69	2 (20%)
3	SO4	B	1002	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	1002	-	4,4,4	0.22	0	6,6,6	0.20	0
3	SO4	C	1002	-	4,4,4	0.25	0	6,6,6	0.05	0
3	SO4	C	1003	-	4,4,4	0.24	0	6,6,6	0.12	0
2	MLT	B	1001	-	8,8,8	1.11	0	10,10,10	1.78	3 (30%)
3	SO4	A	1003	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	D	1004	-	4,4,4	0.23	0	6,6,6	0.11	0
4	GOL	D	1005	-	5,5,5	0.93	0	5,5,5	1.07	0
2	MLT	D	1001	-	8,8,8	1.10	0	10,10,10	1.63	2 (20%)
3	SO4	B	1004	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	1003	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	1003	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	C	1004	-	4,4,4	0.23	0	6,6,6	0.05	0
2	MLT	A	1001	-	8,8,8	1.11	0	10,10,10	1.59	2 (20%)
3	SO4	D	1002	-	4,4,4	0.25	0	6,6,6	0.42	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	MLT	C	1001	-	-	3/8/8/8	-
2	MLT	B	1001	-	-	2/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	1005	-	-	2/4/4/4	-
2	MLT	D	1001	-	-	4/8/8/8	-
2	MLT	A	1001	-	-	4/8/8/8	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	MLT	O2-C1-C2	3.68	120.52	112.74
2	C	1001	MLT	O2-C1-C2	3.61	120.37	112.74
2	D	1001	MLT	O2-C1-C2	3.51	120.16	112.74
2	A	1001	MLT	O2-C1-C2	3.48	120.10	112.74
2	C	1001	MLT	O5-C4-C3	2.19	120.80	114.00
2	D	1001	MLT	O5-C4-C3	2.15	120.70	114.00
2	B	1001	MLT	O5-C4-C3	2.09	120.49	114.00
2	B	1001	MLT	C2-C3-C4	-2.08	106.64	112.08
2	A	1001	MLT	O5-C4-C3	2.03	120.32	114.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MLT	O1-C1-C2-O3
2	A	1001	MLT	O2-C1-C2-O3
2	A	1001	MLT	O2-C1-C2-C3
2	B	1001	MLT	O1-C1-C2-O3
2	B	1001	MLT	O2-C1-C2-O3
2	C	1001	MLT	O1-C1-C2-O3
2	C	1001	MLT	O2-C1-C2-O3
4	D	1005	GOL	O1-C1-C2-C3
4	D	1005	GOL	O1-C1-C2-O2
2	D	1001	MLT	O1-C1-C2-O3
2	D	1001	MLT	O2-C1-C2-O3
2	A	1001	MLT	O1-C1-C2-C3
2	C	1001	MLT	O2-C1-C2-C3
2	D	1001	MLT	O1-C1-C2-C3
2	D	1001	MLT	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	SO4	1	0
3	D	1002	SO4	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	919/970 (94%)	0.03	18 (1%) 65 56	37, 62, 91, 118	0
1	B	915/970 (94%)	-0.26	7 (0%) 82 75	23, 48, 81, 107	3 (0%)
1	C	918/970 (94%)	-0.35	13 (1%) 73 64	30, 47, 77, 119	0
1	D	919/970 (94%)	-0.34	12 (1%) 75 66	26, 46, 82, 119	3 (0%)
All	All	3671/3880 (94%)	-0.23	50 (1%) 73 64	23, 50, 85, 119	6 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	ILE	5.2
1	A	365	ILE	4.6
1	B	765	PRO	4.6
1	A	921	PRO	3.4
1	D	365	ILE	3.2
1	C	365	ILE	3.2
1	C	926	SER	3.0
1	A	14	HIS	3.0
1	A	178	PRO	3.0
1	C	765	PRO	2.9
1	D	914	ASP	2.9
1	C	73	GLY	2.9
1	C	923	PRO	2.7
1	A	765	PRO	2.6
1	C	915	PRO	2.6
1	C	228	ASP	2.5
1	A	181	SER	2.5
1	A	179	THR	2.5
1	B	74	LYS	2.5
1	A	347	HIS	2.4
1	D	181	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	234	GLN	2.4
1	A	24	VAL	2.4
1	A	807	ARG	2.4
1	B	761	ALA	2.4
1	C	395	SER	2.4
1	D	765	PRO	2.4
1	D	926	SER	2.3
1	A	869	GLN	2.3
1	B	178	PRO	2.3
1	D	75	GLY	2.3
1	D	233	ALA	2.3
1	D	178	PRO	2.3
1	C	178	PRO	2.2
1	A	919	VAL	2.2
1	A	183	ARG	2.2
1	B	13	HIS	2.2
1	A	915	PRO	2.2
1	A	926	SER	2.2
1	A	233	ALA	2.2
1	D	580[A]	ARG	2.1
1	A	12	LYS	2.1
1	B	250	GLU	2.1
1	C	924	PRO	2.1
1	D	915	PRO	2.1
1	A	13	HIS	2.0
1	C	383	TYR	2.0
1	D	347	HIS	2.0
1	C	346	LEU	2.0
1	C	159	GLU	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

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($\text{\AA}^2$)	Q<0.9
3	SO4	A	1003	5/5	0.62	0.14	124,124,129,132	0
3	SO4	B	1003	5/5	0.67	0.14	102,116,129,130	0
3	SO4	C	1002	5/5	0.81	0.13	98,100,112,126	0
3	SO4	B	1004	5/5	0.83	0.14	104,105,113,118	0
3	SO4	D	1003	5/5	0.83	0.18	92,101,106,121	0
3	SO4	C	1003	5/5	0.85	0.18	83,89,95,103	0
3	SO4	C	1004	5/5	0.86	0.13	101,106,113,115	0
3	SO4	A	1002	5/5	0.87	0.15	94,97,101,104	0
3	SO4	B	1002	5/5	0.88	0.17	89,91,96,99	0
3	SO4	D	1002	5/5	0.89	0.16	77,87,95,97	0
3	SO4	D	1004	5/5	0.91	0.09	80,91,95,100	0
2	MLT	B	1001	9/9	0.92	0.13	41,49,53,53	0
2	MLT	D	1001	9/9	0.94	0.09	40,43,50,51	0
4	GOL	D	1005	6/6	0.94	0.13	68,71,82,93	0
2	MLT	C	1001	9/9	0.95	0.09	43,48,52,61	0
2	MLT	A	1001	9/9	0.95	0.08	51,61,62,68	0

6.5 Other polymers

There are no such residues in this entry.