



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 01:48 AM EDT

PDB ID : 3E3L
Title : The R-state Glycogen Phosphorylase
Authors : Leonidas, D.D.; Zographos, S.E.; Oikonomakos, N.G.
Deposited on : unknown
Resolution : 2.59 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

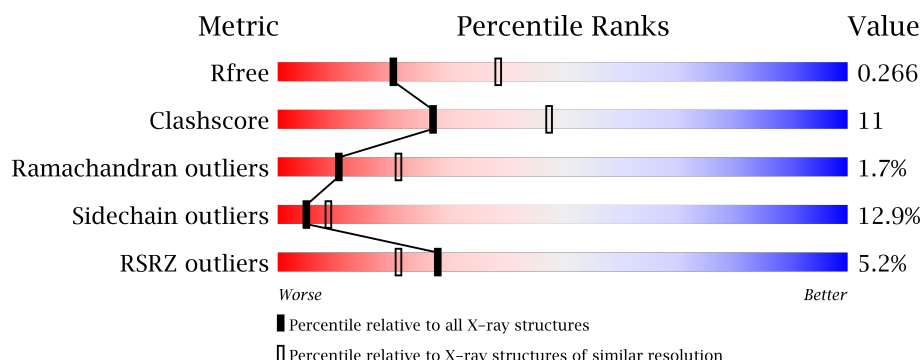
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	842	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>5%</div> <div></div> </div> </div>
1	B	842	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div></div> </div> </div>
1	C	842	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div></div> </div> </div>
1	D	842	<div> <div>7%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>6%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	901	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26533 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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	P	S	0	0	0
			6601	4206	1164	1201	1	29			
1	B	811	Total	C	N	O	P	S	0	0	0
			6608	4208	1165	1205	1	29			
1	C	807	Total	C	N	O	P	S	0	0	0
			6578	4192	1161	1195	1	29			
1	D	806	Total	C	N	O	P	S	0	0	0
			6576	4190	1159	1197	1	29			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

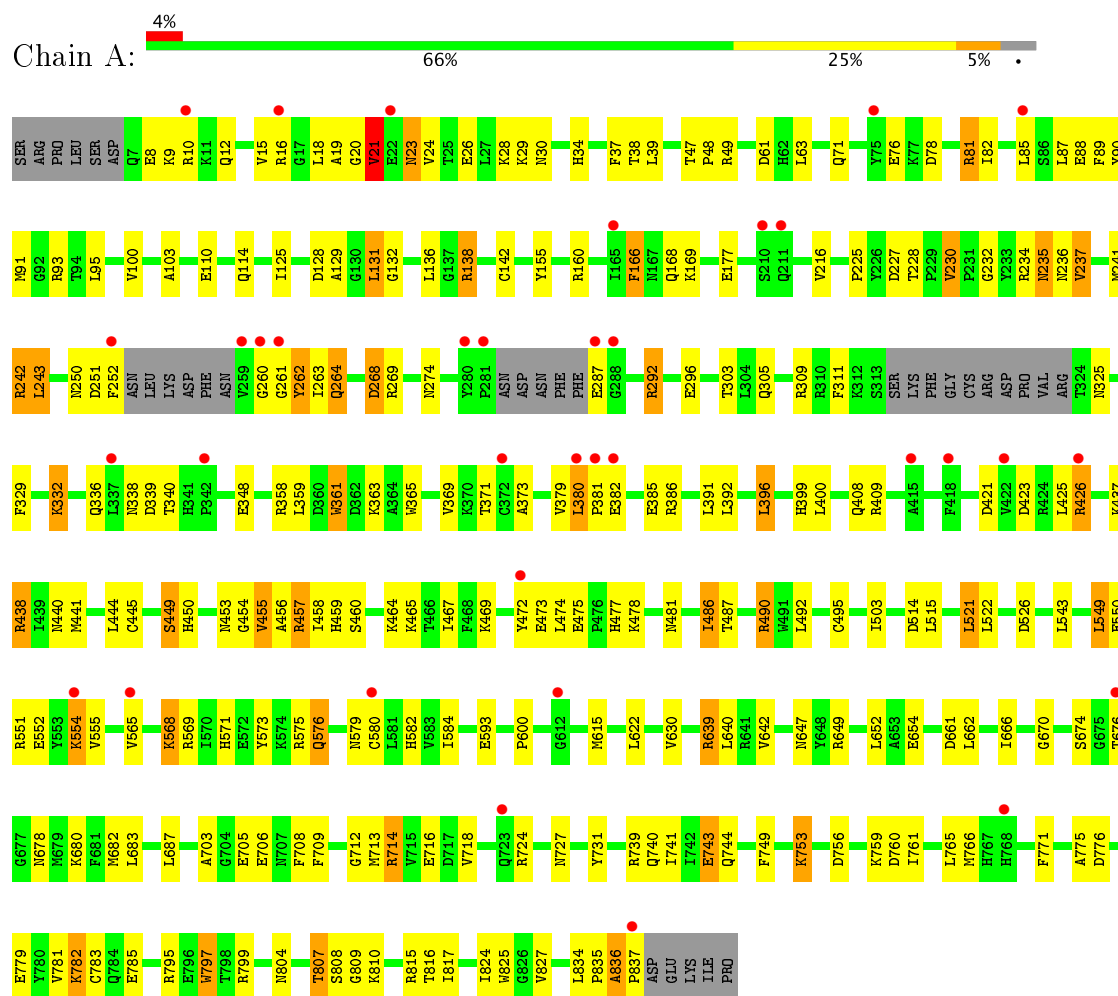
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	35	Total	O	0	0
			35	35		
3	C	26	Total	O	0	0
			26	26		
3	D	26	Total	O	0	0
			26	26		

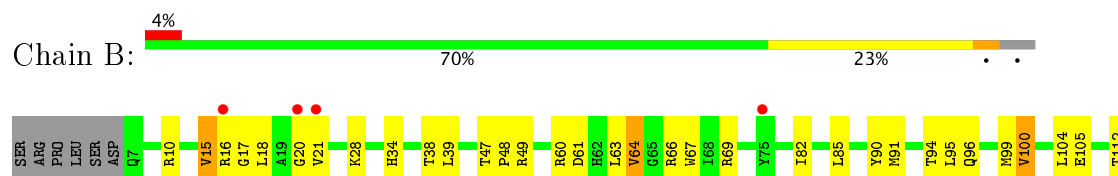
3 Residue-property plots

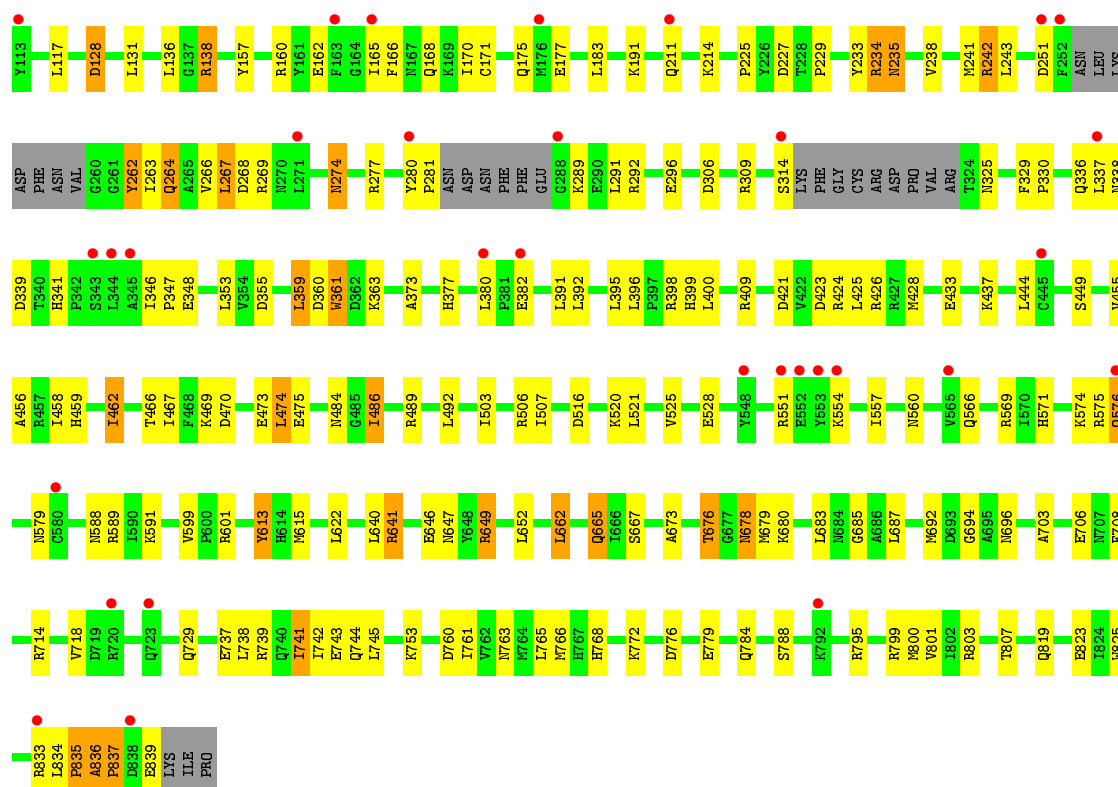
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Glycogen phosphorylase, muscle form

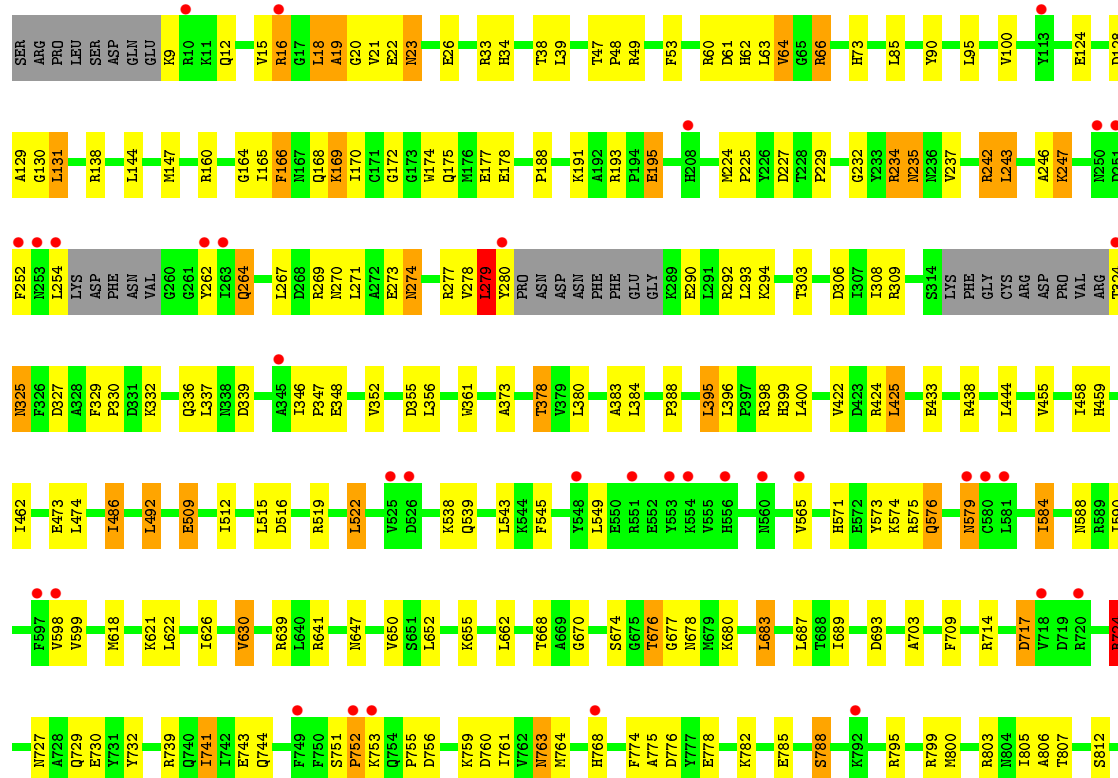


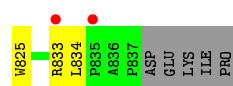
- Molecule 1: Glycogen phosphorylase, muscle form



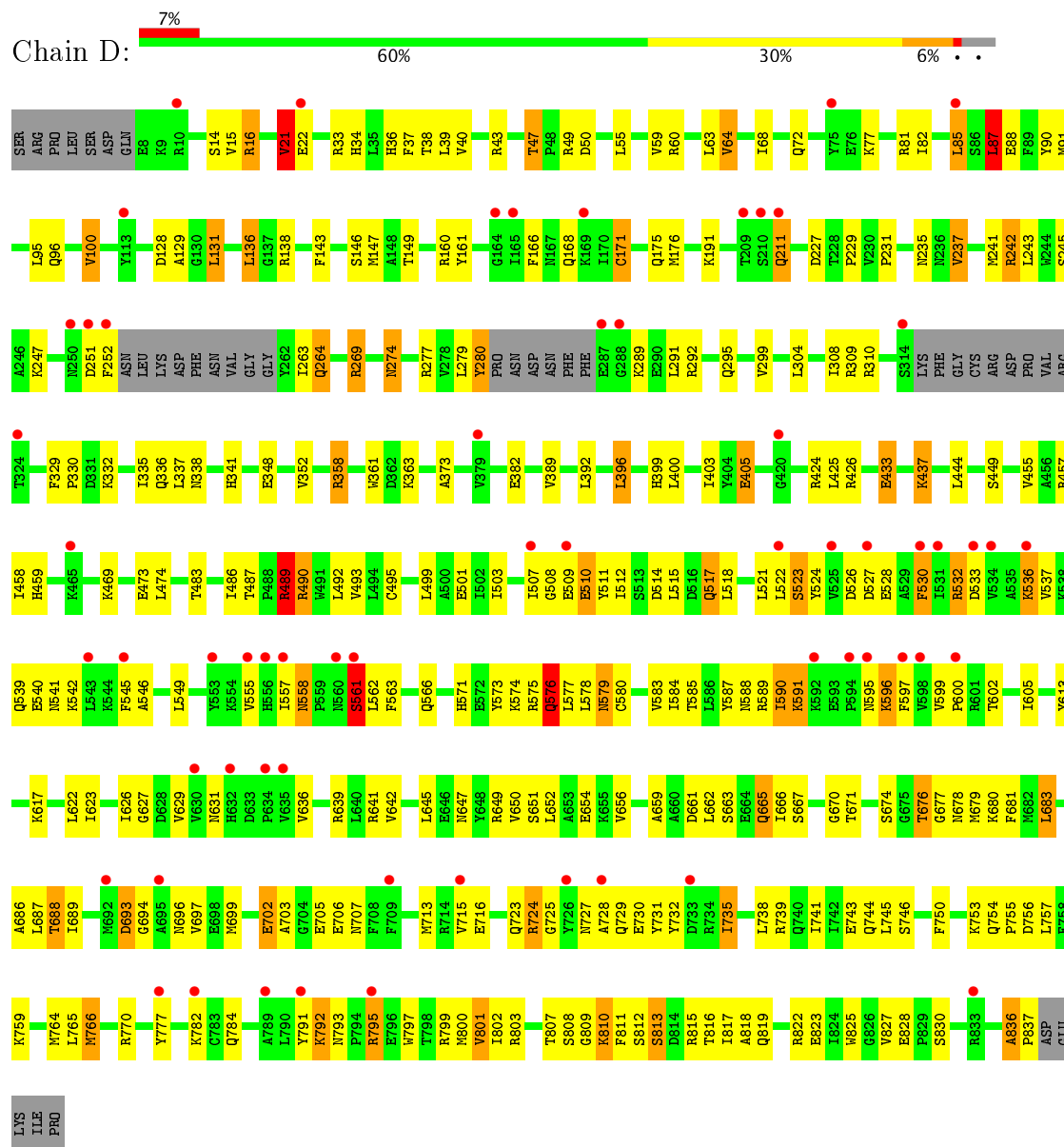


• Molecule 1: Glycogen phosphorylase, muscle form





● Molecule 1: Glycogen phosphorylase, muscle form



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.89Å 189.92Å 88.16Å 90.00° 109.27° 90.00°	Depositor
Resolution (Å)	29.59 – 2.59 29.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.59-2.59) 99.4 (29.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.266 0.207 , 0.266	Depositor DCC
R_{free} test set	5654 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26533	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: LLP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.49	0/6721	0.66	0/9091
1	B	0.49	0/6728	0.66	1/9100 (0.0%)
1	C	0.50	1/6697 (0.0%)	0.66	2/9058 (0.0%)
1	D	0.50	0/6695	0.66	1/9055 (0.0%)
All	All	0.49	1/26841 (0.0%)	0.66	4/36304 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	795	ARG	CZ-NH1	6.38	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	795	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	87	LEU	CA-CB-CG	-5.98	101.54	115.30
1	C	279	LEU	CA-CB-CG	5.30	127.48	115.30
1	B	662	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	VAL	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	6601	0	6554	153	0
1	B	6608	0	6554	116	0
1	C	6578	0	6537	138	0
1	D	6576	0	6528	203	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	20	0	0	1	0
3	A	23	0	0	0	0
3	B	35	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	1	0
All	All	26533	0	26173	597	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 11.

All (597) 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:712:GLY:H	1:A:779:GLU:HG2	1.22	1.03
1:B:641:ARG:HH11	1:B:641:ARG:HG3	1.24	0.98
1:A:20:GLY:O	1:A:21:VAL:HG13	1.65	0.96
1:D:707:ASN:HA	1:D:800:MET:SD	2.09	0.93
1:C:274:ASN:HD22	1:C:274:ASN:H	1.18	0.92
1:D:146:SER:OG	1:D:813:SER:HB2	1.66	0.92
1:D:588:ASN:HD21	1:D:744:GLN:HE22	1.00	0.91
1:C:138:ARG:O	1:C:138:ARG:HD3	1.70	0.90
1:B:455:VAL:H	1:B:459:HIS:HD2	1.18	0.88
1:C:66:ARG:HG3	1:C:66:ARG:HH11	1.39	0.87
1:A:682:MET:HE3	1:A:808:SER:HB2	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:THR:HG22	1:B:680:LLP:H4'1	1.58	0.86
1:A:262:TYR:HB3	1:A:264:GLN:NE2	1.91	0.86
1:A:93:ARG:O	1:A:490:ARG:NH2	2.08	0.86
1:A:227:ASP:OD1	1:A:242:ARG:HD3	1.76	0.85
1:C:516:ASP:O	1:C:519:ARG:HG2	1.76	0.85
1:C:455:VAL:CG1	1:C:674:SER:HB2	2.09	0.83
1:A:87:LEU:HD21	1:A:292:ARG:NH2	1.94	0.83
1:A:703:ALA:HA	1:A:807:THR:HG21	1.60	0.82
1:A:426:ARG:HH21	1:D:755:PRO:HD3	1.45	0.81
1:D:455:VAL:HG12	1:D:674:SER:HB2	1.63	0.81
1:C:274:ASN:H	1:C:274:ASN:ND2	1.79	0.81
1:A:615:MET:CE	1:A:761:ILE:HG12	2.11	0.81
1:D:495:CYS:HB2	1:D:654:GLU:O	1.81	0.81
1:C:703:ALA:HA	1:C:807:THR:HG21	1.63	0.80
1:B:687:LEU:HD13	1:B:800:MET:HE2	1.63	0.80
1:B:486:ILE:HD11	1:B:676:THR:HG23	1.64	0.79
1:C:739:ARG:O	1:C:743:GLU:HG2	1.82	0.79
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.17	0.79
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.46	0.79
1:D:836:ALA:HB1	1:D:837:PRO:HA	1.65	0.79
1:D:739:ARG:O	1:D:743:GLU:HG2	1.83	0.78
1:A:682:MET:CE	1:A:808:SER:HB2	2.12	0.78
1:B:641:ARG:CG	1:B:641:ARG:HH11	1.96	0.78
1:A:168:GLN:HE21	1:A:647:ASN:H	1.28	0.77
1:D:588:ASN:HD21	1:D:744:GLN:NE2	1.81	0.77
1:B:47:THR:HG22	1:B:49:ARG:H	1.50	0.76
1:B:227:ASP:OD1	1:B:242:ARG:HD3	1.84	0.76
1:D:813:SER:O	1:D:817:ILE:HG12	1.85	0.76
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.51	0.76
1:B:703:ALA:HA	1:B:807:THR:HG21	1.66	0.76
1:A:110:GLU:HG3	1:A:114:GLN:HE21	1.50	0.75
1:D:588:ASN:ND2	1:D:744:GLN:HE22	1.80	0.75
1:C:168:GLN:HG3	1:C:175:GLN:HG3	1.67	0.75
1:D:665:GLN:HB3	1:D:696:ASN:HD21	1.52	0.75
1:D:455:VAL:CG1	1:D:674:SER:HB2	2.15	0.75
1:A:262:TYR:HB3	1:A:264:GLN:HE22	1.53	0.74
1:A:455:VAL:H	1:A:459:HIS:HD2	1.35	0.74
1:C:47:THR:HG23	1:C:48:PRO:HD2	1.70	0.74
1:C:274:ASN:N	1:C:274:ASN:HD22	1.82	0.74
1:C:588:ASN:HD21	1:C:744:GLN:HE22	1.37	0.73
1:C:741:ILE:HA	1:C:744:GLN:HE21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:VAL:H	1:D:459:HIS:HD2	1.36	0.73
1:A:739:ARG:O	1:A:743:GLU:HG2	1.89	0.72
1:B:455:VAL:H	1:B:459:HIS:CD2	2.06	0.72
1:C:60:ARG:O	1:C:64:VAL:HG13	1.90	0.72
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.70	0.71
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.73	0.71
1:B:729:GLN:HG2	1:C:724:ARG:HA	1.73	0.71
1:C:574:LYS:HB2	1:C:576:GLN:HE22	1.53	0.71
1:A:47:THR:HG22	1:A:49:ARG:H	1.57	0.70
1:A:712:GLY:N	1:A:779:GLU:HG2	2.01	0.70
1:B:168:GLN:HE21	1:B:647:ASN:H	1.39	0.70
1:C:235:ASN:HD22	1:C:235:ASN:H	1.38	0.70
1:A:438:ARG:HH11	1:A:438:ARG:CG	2.05	0.70
1:A:582:HIS:HD2	1:A:781:VAL:HG12	1.54	0.70
1:A:269:ARG:HH21	1:B:277:ARG:HH22	1.36	0.70
1:B:336:GLN:NE2	1:B:373:ALA:HB3	2.08	0.69
1:D:800:MET:C	1:D:802:ILE:H	1.96	0.68
1:A:756:ASP:HB2	1:A:759:LYS:HG3	1.75	0.68
1:A:615:MET:HE3	1:A:761:ILE:HG12	1.75	0.68
1:C:227:ASP:OD1	1:C:242:ARG:HD3	1.94	0.68
1:C:308:ILE:HD12	1:C:352:VAL:HG11	1.75	0.68
1:A:21:VAL:HG21	1:A:26:GLU:HG3	1.74	0.68
1:C:47:THR:HG22	1:C:49:ARG:H	1.58	0.67
1:C:378:THR:HG21	1:C:383:ALA:HB3	1.76	0.67
1:B:458:ILE:O	1:B:462:ILE:HG12	1.95	0.67
1:A:168:GLN:NE2	1:A:647:ASN:H	1.93	0.66
1:A:703:ALA:CA	1:A:807:THR:HG21	2.25	0.66
1:D:800:MET:O	1:D:802:ILE:N	2.27	0.66
1:B:741:ILE:HA	1:B:744:GLN:HE21	1.60	0.66
1:C:252:PHE:HZ	1:C:269:ARG:HB2	1.59	0.66
1:D:801:VAL:HG12	1:D:801:VAL:O	1.95	0.66
1:C:144:LEU:HD23	1:C:147:MET:CE	2.26	0.65
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.10	0.65
1:D:681:PHE:O	1:D:686:ALA:HB3	1.96	0.65
1:A:250:ASN:HB3	1:A:252:PHE:HE2	1.62	0.65
1:B:100:VAL:O	1:B:234:ARG:NH1	2.29	0.65
1:D:689:ILE:HG23	1:D:689:ILE:O	1.97	0.65
1:A:365:TRP:O	1:A:369:VAL:HG23	1.96	0.65
1:B:157:TYR:OH	1:B:306:ASP:OD2	2.13	0.65
1:B:280:TYR:HD1	1:B:281:PRO:HA	1.62	0.64
1:A:138:ARG:O	1:A:138:ARG:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ASP:OD1	1:B:309:ARG:NH1	2.31	0.64
1:D:14:SER:OG	1:D:16:ARG:HG2	1.97	0.64
1:D:627:GLY:HA2	1:D:642:VAL:HB	1.80	0.64
1:D:590:ILE:O	1:D:590:ILE:HG22	1.98	0.64
1:C:262:TYR:HB2	1:C:264:GLN:OE1	1.97	0.64
1:D:60:ARG:O	1:D:64:VAL:HG12	1.98	0.63
1:A:795:ARG:O	1:A:799:ARG:HG3	1.99	0.63
1:D:211:GLN:HG3	1:D:358:ARG:NH2	2.13	0.63
1:C:21:VAL:HG22	1:C:22:GLU:HG2	1.80	0.63
1:D:146:SER:HG	1:D:813:SER:HB2	1.62	0.63
1:C:378:THR:CG2	1:C:383:ALA:HB3	2.29	0.63
1:C:455:VAL:H	1:C:459:HIS:HD2	1.45	0.63
1:D:455:VAL:N	1:D:459:HIS:HD2	1.97	0.63
1:C:676:THR:HG22	1:C:680:LLP:H5'1	1.82	0.62
1:A:445:CYS:O	1:A:449:SER:OG	2.17	0.62
1:D:741:ILE:HA	1:D:744:GLN:HE21	1.64	0.62
1:D:661:ASP:HB3	1:D:797:TRP:CH2	2.34	0.62
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.15	0.62
1:D:574:LYS:HB3	1:D:576:GLN:NE2	2.15	0.62
1:D:507:ILE:HD12	1:D:517:GLN:HG2	1.81	0.62
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.83	0.61
1:A:49:ARG:HA	1:A:125:ILE:HG21	1.83	0.61
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.82	0.61
1:B:687:LEU:HD13	1:B:800:MET:CE	2.30	0.61
1:B:803:ARG:O	1:B:807:THR:HG22	2.01	0.61
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.82	0.61
1:B:15:VAL:HA	1:B:18:LEU:HD22	1.81	0.61
1:D:801:VAL:O	1:D:801:VAL:CG1	2.49	0.60
1:C:424:ARG:NH2	1:C:473:GLU:OE1	2.35	0.60
1:A:110:GLU:HG3	1:A:114:GLN:NE2	2.17	0.60
1:A:582:HIS:CD2	1:A:781:VAL:HG12	2.36	0.60
1:A:549:LEU:O	1:A:552:GLU:O	2.20	0.59
1:D:566:GLN:HE22	1:D:576:GLN:HA	1.66	0.59
1:C:509:GLU:HG2	1:C:512:ILE:HD12	1.82	0.59
1:D:599:VAL:HG12	1:D:600:PRO:O	2.03	0.59
1:D:563:PHE:HD2	1:D:659:ALA:O	1.85	0.59
1:A:680:LLP:O3	1:A:680:LLP:NZ	2.36	0.59
1:B:225:PRO:HB2	1:B:242:ARG:HD2	1.84	0.59
1:D:600:PRO:HB3	1:D:639:ARG:HA	1.83	0.59
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.83	0.59
1:C:165:ILE:O	1:C:166:PHE:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:539:GLN:C	1:D:541:ASN:H	2.06	0.59
1:D:662:LEU:HD23	1:D:687:LEU:O	2.02	0.59
1:B:96:GLN:HA	1:B:99:MET:HE2	1.85	0.59
1:C:579:ASN:C	1:C:579:ASN:HD22	2.06	0.58
1:A:296:GLU:OE2	1:A:385:GLU:OE2	2.21	0.58
1:A:9:LYS:H	1:A:9:LYS:HD2	1.69	0.58
1:D:580:CYS:O	1:D:584:ILE:HG13	2.03	0.58
1:C:574:LYS:HB2	1:C:576:GLN:NE2	2.18	0.58
1:D:676:THR:HG22	1:D:680:LLP:H5'1	1.84	0.58
1:D:21:VAL:CG2	1:D:22:GLU:N	2.67	0.58
1:C:270:ASN:O	1:C:274:ASN:ND2	2.37	0.58
1:D:348:GLU:OE1	1:D:399:HIS:HE1	1.87	0.58
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.85	0.57
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.03	0.57
1:D:573:TYR:HD2	1:D:671:THR:HG1	1.52	0.57
1:A:311:PHE:CG	1:A:311:PHE:O	2.57	0.57
1:C:33:ARG:HE	1:D:33:ARG:NE	2.03	0.57
1:A:336:GLN:HG2	1:A:825:TRP:HE1	1.70	0.57
1:C:279:LEU:HD22	1:C:280:TYR:H	1.70	0.57
1:D:129:ALA:HB1	1:D:131:LEU:HD22	1.87	0.57
1:D:651:SER:HA	1:D:654:GLU:HG2	1.86	0.57
1:A:110:GLU:O	1:A:114:GLN:HG2	2.05	0.57
1:B:615:MET:HE3	1:B:761:ILE:HG12	1.87	0.57
1:B:105:GLU:OE1	1:B:105:GLU:HA	2.04	0.57
1:B:615:MET:CE	1:B:761:ILE:HG12	2.34	0.57
1:A:426:ARG:HB2	1:A:426:ARG:CZ	2.33	0.57
1:A:457:ARG:CG	1:A:457:ARG:HH11	2.18	0.57
1:D:87:LEU:HD13	1:D:341:HIS:HB3	1.87	0.57
1:C:64:VAL:HG22	1:D:37:PHE:HD1	1.70	0.56
1:A:87:LEU:HD21	1:A:292:ARG:HH22	1.68	0.56
1:D:579:ASN:HD22	1:D:605:ILE:HD11	1.70	0.56
1:D:702:GLU:HA	1:D:702:GLU:OE2	2.04	0.56
1:A:815:ARG:NH1	1:A:816:THR:HA	2.19	0.56
1:D:584:ILE:HG22	1:D:741:ILE:HG22	1.86	0.56
1:A:554:LYS:HD3	1:A:554:LYS:N	2.20	0.56
1:B:391:LEU:O	1:B:395:LEU:HD23	2.06	0.56
1:D:663:SER:HB2	1:D:681:PHE:HB3	1.88	0.56
1:D:455:VAL:H	1:D:459:HIS:CD2	2.21	0.56
1:D:47:THR:HG22	1:D:50:ASP:H	1.69	0.56
1:A:336:GLN:NE2	1:A:373:ALA:HB3	2.21	0.55
1:D:574:LYS:HB3	1:D:576:GLN:HE22	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:GLN:HE21	1:D:825:TRP:HE1	1.54	0.55
1:A:824:ILE:HG22	1:A:825:TRP:CD1	2.41	0.55
1:A:782:LYS:HE3	1:A:782:LYS:HA	1.88	0.55
1:D:702:GLU:CA	1:D:702:GLU:OE2	2.54	0.55
1:A:486:ILE:CD1	1:A:676:THR:O	2.55	0.55
1:B:678:ASN:HB3	1:B:679:MET:HG3	1.89	0.55
1:D:21:VAL:HG22	1:D:22:GLU:N	2.22	0.55
1:D:703:ALA:O	1:D:707:ASN:ND2	2.40	0.55
1:B:227:ASP:OD1	1:B:242:ARG:CD	2.54	0.55
1:D:149:THR:HG21	1:D:489:ARG:HH12	1.70	0.55
1:B:280:TYR:CD1	1:B:281:PRO:HA	2.41	0.55
1:C:756:ASP:HB2	1:C:759:LYS:HD2	1.89	0.55
1:B:346:ILE:HB	1:B:347:PRO:HD3	1.89	0.54
1:B:718:VAL:HG13	1:B:772:LYS:HZ2	1.72	0.54
1:C:486:ILE:HD11	1:C:680:LLP:HE2	1.88	0.54
1:A:166:PHE:CD2	1:A:177:GLU:HB3	2.42	0.54
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.43	0.54
1:A:455:VAL:HG13	1:A:674:SER:HB2	1.89	0.54
1:D:670:GLY:H	1:D:693:ASP:CG	2.10	0.54
1:B:168:GLN:NE2	1:B:647:ASN:H	2.03	0.54
1:D:160:ARG:HB2	1:D:243:LEU:HB3	1.88	0.54
1:C:599:VAL:HG21	1:C:788:SER:O	2.07	0.54
1:D:241:MET:HG2	1:D:243:LEU:HD13	1.89	0.54
1:A:88:GLU:HB3	1:A:132:GLY:HA2	1.90	0.54
1:B:136:LEU:HD23	1:B:338:ASN:ND2	2.23	0.54
1:D:689:ILE:HD12	1:D:784:GLN:OE1	2.07	0.54
1:B:685:GLY:HA2	1:B:801:VAL:HG13	1.89	0.54
1:B:474:LEU:HD13	1:B:475:GLU:HG3	1.90	0.53
1:C:252:PHE:CZ	1:C:269:ARG:HB2	2.41	0.53
1:D:791:TYR:C	1:D:793:ASN:H	2.10	0.53
1:D:274:ASN:HB2	1:D:277:ARG:HD3	1.89	0.53
1:D:800:MET:C	1:D:802:ILE:N	2.62	0.53
1:C:271:LEU:HA	1:C:274:ASN:HD21	1.73	0.53
1:D:558:ASN:O	1:D:561:SER:HB2	2.08	0.53
1:D:636:VAL:O	1:D:639:ARG:HG3	2.08	0.53
1:C:306:ASP:OD1	1:C:309:ARG:NH1	2.41	0.53
1:C:34:HIS:HE1	1:C:61:ASP:OD2	1.91	0.53
1:C:232:GLY:HA3	1:C:235:ASN:HD21	1.74	0.53
1:D:143:PHE:HB3	1:D:147:MET:HE2	1.90	0.53
1:D:68:ILE:O	1:D:72:GLN:HG3	2.08	0.53
1:B:112:THR:HG22	1:B:117:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ASN:HD21	1:B:744:GLN:HE22	1.54	0.53
1:C:522:LEU:HD22	1:C:806:ALA:HB1	1.90	0.53
1:C:66:ARG:CG	1:C:66:ARG:HH11	2.16	0.53
1:C:680:LLP:O3	1:C:680:LLP:NZ	2.42	0.53
1:C:764:MET:HA	1:C:768:HIS:CE1	2.44	0.53
1:A:264:GLN:HE21	1:A:264:GLN:H	1.56	0.53
1:B:738:LEU:O	1:B:742:ILE:HG12	2.08	0.53
1:D:136:LEU:HD22	1:D:338:ASN:HD21	1.73	0.53
1:D:235:ASN:CG	1:D:237:VAL:HG13	2.30	0.53
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.49	0.52
1:B:834:LEU:O	1:B:835:PRO:O	2.27	0.52
1:C:455:VAL:HG12	1:C:674:SER:HB2	1.89	0.52
1:D:171:CYS:SG	1:D:176:MET:HG3	2.49	0.52
1:D:533:ASP:HA	1:D:536:LYS:HB3	1.91	0.52
1:B:641:ARG:NH1	1:B:641:ARG:HG3	2.05	0.52
1:D:589:ARG:O	1:D:591:LYS:N	2.33	0.52
1:D:63:LEU:HD13	1:D:229:PRO:HG2	1.92	0.52
1:B:353:LEU:O	1:B:359:LEU:HB2	2.08	0.52
1:A:575:ARG:NH2	1:A:776:ASP:HB2	2.23	0.52
1:A:237:VAL:HG12	1:A:834:LEU:HD13	1.92	0.52
1:C:455:VAL:H	1:C:459:HIS:CD2	2.26	0.52
1:C:235:ASN:ND2	1:C:235:ASN:H	2.06	0.52
1:A:676:THR:HG23	1:A:680:LLP:H4'1	1.92	0.52
1:A:554:LYS:HD3	1:A:554:LYS:H	1.75	0.52
1:B:466:THR:OG1	1:B:467:ILE:HD12	2.10	0.52
1:C:168:GLN:HE21	1:C:647:ASN:H	1.56	0.52
1:D:663:SER:OG	1:D:688:THR:HG23	2.10	0.52
1:D:308:ILE:HD13	1:D:352:VAL:HG11	1.92	0.52
1:D:728:ALA:HB3	1:D:766:MET:O	2.10	0.52
1:C:224:MET:SD	1:C:247:LYS:HE3	2.49	0.51
1:C:590:ILE:HG12	1:C:598:VAL:HG11	1.92	0.51
1:D:503:ILE:HG23	1:D:521:LEU:HD11	1.92	0.51
1:D:815:ARG:O	1:D:819:GLN:HG3	2.10	0.51
1:D:595:ASN:O	1:D:596:LYS:C	2.48	0.51
1:A:703:ALA:CB	1:A:807:THR:HG21	2.41	0.51
1:B:241:MET:HG2	1:B:243:LEU:HD13	1.91	0.51
1:D:584:ILE:HG23	1:D:750:PHE:HZ	1.76	0.51
1:A:486:ILE:HD11	1:A:676:THR:O	2.10	0.51
1:D:336:GLN:NE2	1:D:825:TRP:HE1	2.09	0.51
1:A:687:LEU:HD12	1:A:797:TRP:CE2	2.45	0.51
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.94	0.51
1:B:16:ARG:HG3	1:B:17:GLY:H	1.76	0.51
1:B:426:ARG:CZ	1:C:755:PRO:HD2	2.40	0.51
1:D:580:CYS:SG	1:D:623:ILE:HG12	2.51	0.51
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.76	0.51
1:B:433:GLU:OE2	1:B:437:LYS:HE2	2.11	0.51
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.11	0.51
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.75	0.50
1:D:508:GLY:O	1:D:510:GLU:N	2.45	0.50
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.74	0.50
1:A:379:VAL:HG21	1:A:670:GLY:O	2.10	0.50
1:B:680:LLP:NZ	1:B:680:LLP:O3	2.44	0.50
1:A:23:ASN:HB3	1:A:26:GLU:HG2	1.92	0.50
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.94	0.50
1:C:246:ALA:C	1:C:247:LYS:HG2	2.32	0.50
1:D:571:HIS:CD2	1:D:613:TYR:HE2	2.29	0.50
1:A:78:ASP:OD2	1:A:332:LYS:NZ	2.44	0.50
1:A:573:TYR:HB3	1:A:771:PHE:CE1	2.47	0.50
1:C:169:LYS:NZ	1:C:178:GLU:OE1	2.45	0.50
1:D:263:ILE:HG13	1:D:263:ILE:O	2.12	0.50
1:D:336:GLN:HE22	1:D:373:ALA:HB3	1.76	0.50
1:D:63:LEU:HD21	1:D:231:PRO:HB3	1.94	0.50
1:A:575:ARG:HD3	1:A:666:ILE:O	2.12	0.50
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.95	0.50
1:A:661:ASP:HB3	1:A:797:TRP:CH2	2.47	0.50
1:C:324:THR:O	1:C:325:ASN:O	2.30	0.50
1:C:34:HIS:HD2	1:C:38:THR:OG1	1.95	0.50
1:A:20:GLY:O	1:A:21:VAL:CG1	2.51	0.49
1:A:386:ARG:HG2	1:A:440:ASN:HA	1.93	0.49
1:D:280:TYR:OH	1:D:291:LEU:HD12	2.12	0.49
1:D:661:ASP:HB3	1:D:797:TRP:HH2	1.74	0.49
1:B:395:LEU:HD23	1:B:395:LEU:H	1.77	0.49
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.94	0.49
1:D:818:ALA:O	1:D:822:ARG:HG3	2.12	0.49
1:A:235:ASN:HD22	1:A:236:ASN:N	2.10	0.49
1:B:348:GLU:OE1	1:B:399:HIS:CE1	2.65	0.49
1:D:21:VAL:CG2	1:D:22:GLU:H	2.25	0.49
1:D:85:LEU:HD12	1:D:335:ILE:HG23	1.93	0.49
1:C:741:ILE:HA	1:C:744:GLN:NE2	2.26	0.49
1:D:575:ARG:C	1:D:577:LEU:N	2.65	0.49
1:C:336:GLN:HE21	1:C:825:TRP:HE1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLU:HA	1:B:183:LEU:HD12	1.94	0.49
1:C:676:THR:HG22	1:C:680:LLP:H4'1	1.94	0.49
1:D:584:ILE:HG23	1:D:750:PHE:CZ	2.47	0.49
1:A:142:CYS:SG	1:A:487:THR:HG22	2.52	0.49
1:D:545:PHE:O	1:D:549:LEU:HB2	2.12	0.49
1:A:227:ASP:OD1	1:A:242:ARG:CD	2.56	0.49
1:A:241:MET:HG2	1:A:243:LEU:HD13	1.95	0.49
1:A:24:VAL:O	1:A:28:LYS:HG3	2.12	0.49
1:A:740:GLN:O	1:A:744:GLN:HG3	2.12	0.49
1:D:405:GLU:OE1	1:D:405:GLU:HA	2.13	0.49
1:A:731:TYR:CE1	1:A:775:ALA:HA	2.48	0.49
1:B:528:GLU:OE1	1:B:795:ARG:NH1	2.45	0.49
1:C:346:ILE:HB	1:C:347:PRO:HD3	1.95	0.49
1:D:96:GLN:O	1:D:100:VAL:HG13	2.13	0.49
1:A:456:ALA:C	1:A:481:ASN:HD21	2.15	0.49
1:A:474:LEU:O	1:A:475:GLU:HG3	2.12	0.49
1:C:63:LEU:HD13	1:C:229:PRO:HG2	1.95	0.48
1:A:340:THR:OG1	1:A:385:GLU:HB2	2.13	0.48
1:D:389:VAL:HG22	1:D:437:LYS:O	2.12	0.48
1:D:589:ARG:C	1:D:591:LYS:H	2.15	0.48
1:A:309:ARG:NH2	2:A:902:SO4:O1	2.46	0.48
1:C:193:ARG:HB2	1:C:225:PRO:HG2	1.96	0.48
1:C:23:ASN:HB3	1:C:26:GLU:HB2	1.94	0.48
1:A:455:VAL:H	1:A:459:HIS:CD2	2.22	0.48
1:D:168:GLN:NE2	1:D:647:ASN:H	2.12	0.48
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.78	0.48
1:A:47:THR:HG22	1:A:49:ARG:N	2.26	0.48
1:A:568:LYS:NZ	1:A:680:LLP:OP1	2.47	0.48
1:D:424:ARG:NH2	1:D:473:GLU:OE1	2.47	0.48
1:D:836:ALA:CB	1:D:837:PRO:HA	2.37	0.48
1:D:85:LEU:CD1	1:D:335:ILE:HG23	2.44	0.48
1:A:103:ALA:HB2	1:A:234:ARG:HE	1.78	0.48
1:C:170:ILE:HA	1:C:174:TRP:O	2.14	0.48
1:C:336:GLN:NE2	1:C:825:TRP:HE1	2.12	0.48
1:D:348:GLU:OE1	1:D:399:HIS:CE1	2.67	0.48
1:B:428:MET:SD	1:B:470:ASP:HB3	2.54	0.47
1:C:378:THR:HG22	1:C:380:LEU:H	1.79	0.47
1:D:146:SER:HB2	1:D:817:ILE:HG13	1.96	0.47
1:B:739:ARG:O	1:B:743:GLU:HG2	2.14	0.47
1:C:670:GLY:H	1:C:693:ASP:CG	2.17	0.47
1:D:549:LEU:HD23	1:D:557:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASN:OD1	1:B:377:HIS:CE1	2.68	0.47
1:C:324:THR:O	1:C:325:ASN:C	2.53	0.47
1:D:274:ASN:C	1:D:274:ASN:HD22	2.18	0.47
1:C:727:ASN:HD21	1:C:729:GLN:HB3	1.79	0.47
1:A:526:ASP:OD1	1:A:799:ARG:NH1	2.48	0.47
1:B:274:ASN:HA	1:B:277:ARG:HB2	1.95	0.47
1:C:130:GLY:O	1:C:164:GLY:HA2	2.14	0.47
1:C:269:ARG:NH1	1:C:273:GLU:OE1	2.43	0.47
1:C:274:ASN:HA	1:C:277:ARG:HB2	1.97	0.47
1:B:507:ILE:HG21	1:B:520:LYS:HB3	1.96	0.47
1:D:732:TYR:HB2	1:D:766:MET:HE1	1.97	0.47
1:A:23:ASN:HA	1:A:23:ASN:HD22	1.58	0.47
1:A:727:ASN:HD21	1:D:725:GLY:HA3	1.80	0.47
1:B:373:ALA:HA	1:B:449:SER:HB3	1.97	0.46
1:B:128:ASP:OD2	1:B:649:ARG:HG3	2.15	0.46
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.97	0.46
1:B:138:ARG:HD3	1:B:138:ARG:O	2.16	0.46
1:C:336:GLN:HG2	1:C:825:TRP:HE1	1.79	0.46
1:A:380:LEU:HD12	1:A:380:LEU:HA	1.86	0.46
1:A:438:ARG:HG2	1:A:438:ARG:HH11	1.78	0.46
1:D:546:ALA:HA	1:D:549:LEU:HB3	1.98	0.46
1:D:563:PHE:CD1	1:D:602:THR:OG1	2.68	0.46
1:B:336:GLN:HE22	1:B:373:ALA:HB3	1.79	0.46
1:B:462:ILE:HG12	1:B:462:ILE:H	1.62	0.46
1:B:336:GLN:HG2	1:B:825:TRP:HE1	1.79	0.46
1:D:87:LEU:HD13	1:D:341:HIS:CB	2.44	0.46
1:D:43:ARG:NH1	2:D:900:SO4:O1	2.44	0.46
1:A:464:LYS:HG2	1:A:472:TYR:CD1	2.51	0.46
1:D:663:SER:HB3	1:D:688:THR:HA	1.98	0.46
1:D:836:ALA:HB1	1:D:837:PRO:CA	2.40	0.46
1:D:662:LEU:HD22	1:D:689:ILE:HG22	1.98	0.46
1:B:235:ASN:H	1:B:235:ASN:HD22	1.64	0.46
1:B:665:GLN:HB3	1:B:696:ASN:HD21	1.81	0.46
1:D:575:ARG:C	1:D:577:LEU:H	2.19	0.46
1:D:699:MET:HA	1:D:811:PHE:CZ	2.51	0.46
1:C:677:GLY:HA2	1:C:680:LLP:HD3	1.97	0.46
1:D:458:ILE:HD11	1:D:694:GLY:H	1.81	0.46
1:C:47:THR:CG2	1:C:48:PRO:HD2	2.43	0.45
1:D:47:THR:HG23	1:D:49:ARG:H	1.81	0.45
1:D:631:ASN:HA	1:D:641:ARG:NH1	2.31	0.45
1:A:450:HIS:O	1:A:478:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:VAL:O	1:A:785:GLU:HG3	2.16	0.45
1:D:665:GLN:HG2	1:D:678:ASN:OD1	2.16	0.45
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.79	0.45
1:C:66:ARG:HG3	1:C:66:ARG:NH1	2.19	0.45
1:A:438:ARG:NH1	1:A:438:ARG:CG	2.72	0.45
1:A:47:THR:HG23	1:A:48:PRO:HD2	1.98	0.45
1:A:804:ASN:O	1:A:807:THR:HG22	2.15	0.45
1:B:348:GLU:OE1	1:B:399:HIS:HE1	2.00	0.45
1:B:503:ILE:HG23	1:B:521:LEU:HD11	1.99	0.45
1:C:575:ARG:HD2	1:C:668:THR:H	1.81	0.45
1:D:309:ARG:HB3	1:D:309:ARG:HH11	1.82	0.45
1:D:563:PHE:CD2	1:D:659:ALA:O	2.68	0.45
1:D:557:ILE:HG22	1:D:557:ILE:O	2.15	0.45
1:B:557:ILE:HD13	1:B:557:ILE:HA	1.83	0.45
1:C:388:PRO:HA	1:C:438:ARG:HG2	1.98	0.45
1:C:571:HIS:ND1	1:C:573:TYR:HD1	2.15	0.45
1:C:687:LEU:HD22	1:C:800:MET:HE2	1.98	0.45
1:C:618:MET:HB3	1:C:761:ILE:HD11	1.98	0.45
1:D:602:THR:HG22	1:D:641:ARG:HB2	1.99	0.45
1:A:472:TYR:C	1:A:474:LEU:H	2.20	0.45
1:A:550:GLU:HG2	1:A:555:VAL:O	2.16	0.45
1:C:279:LEU:CD2	1:C:280:TYR:H	2.30	0.45
1:A:89:PHE:O	1:A:131:LEU:HB3	2.17	0.45
1:A:348:GLU:OE1	1:A:399:HIS:HE1	2.00	0.45
1:B:47:THR:HG23	1:B:48:PRO:HD2	1.98	0.45
1:B:738:LEU:HD12	1:B:741:ILE:HD11	1.99	0.45
1:A:21:VAL:HG21	1:A:26:GLU:CG	2.43	0.45
1:A:454:GLY:HA3	1:A:460:SER:OG	2.17	0.45
1:C:129:ALA:HB1	1:C:131:LEU:HD22	1.99	0.45
1:C:274:ASN:N	1:C:274:ASN:ND2	2.47	0.45
1:C:584:ILE:HG13	1:C:584:ILE:H	1.67	0.45
1:C:455:VAL:HG13	1:C:674:SER:HB2	1.96	0.45
1:A:456:ALA:C	1:A:481:ASN:ND2	2.70	0.45
1:B:601:ARG:NH2	1:B:784:GLN:OE1	2.46	0.45
1:D:810:LYS:O	1:D:815:ARG:NE	2.34	0.45
1:A:580:CYS:O	1:A:584:ILE:HG13	2.17	0.44
1:C:571:HIS:ND1	1:C:573:TYR:CD1	2.85	0.44
1:A:465:LYS:O	1:A:469:LYS:HD2	2.18	0.44
1:B:16:ARG:HG3	1:B:17:GLY:N	2.33	0.44
1:A:12:GLN:HE22	1:B:28:LYS:HZ2	1.65	0.44
1:B:456:ALA:HB3	1:B:673:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:HB3	1:C:309:ARG:NH1	2.32	0.44
1:D:489:ARG:HE	1:D:489:ARG:H	1.65	0.44
1:B:575:ARG:HH22	1:B:776:ASP:CB	2.29	0.44
1:B:599:VAL:HG21	1:B:788:SER:O	2.17	0.44
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.99	0.44
1:A:810:LYS:O	1:A:810:LYS:HG2	2.16	0.44
1:C:235:ASN:N	1:C:235:ASN:HD22	2.04	0.44
1:C:729:GLN:O	1:C:732:TYR:HB3	2.16	0.44
1:C:799:ARG:O	1:C:803:ARG:HG3	2.18	0.44
1:D:735:ILE:H	1:D:735:ILE:HG12	1.46	0.44
1:C:290:GLU:HG2	1:C:294:LYS:HD2	1.99	0.44
1:B:329:PHE:HB3	1:B:330:PRO:HD3	2.00	0.44
1:D:295:GLN:O	1:D:299:VAL:HG12	2.17	0.44
1:D:650:VAL:HA	1:D:680:LLP:H2'1	2.00	0.44
1:D:803:ARG:HB2	1:D:803:ARG:HE	1.63	0.44
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.99	0.44
1:B:136:LEU:CD2	1:B:338:ASN:ND2	2.80	0.44
1:B:836:ALA:HB1	1:B:837:PRO:HA	2.00	0.44
1:D:493:VAL:HG21	1:D:512:ILE:HG21	2.00	0.44
1:A:753:LYS:N	1:A:753:LYS:HD2	2.33	0.43
1:D:289:LYS:HG3	1:D:291:LEU:H	1.83	0.43
1:C:195:GLU:HG3	1:C:195:GLU:H	1.50	0.43
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.99	0.43
1:D:677:GLY:O	1:D:681:PHE:HD1	2.00	0.43
1:D:754:GLN:HG2	1:D:757:LEU:HD13	2.00	0.43
1:D:495:CYS:HB3	1:D:654:GLU:HB2	2.01	0.43
1:D:699:MET:HA	1:D:811:PHE:HZ	1.82	0.43
1:A:457:ARG:CG	1:A:457:ARG:NH1	2.80	0.43
1:A:817:ILE:HD13	1:A:817:ILE:HA	1.89	0.43
1:B:263:ILE:O	1:B:266:VAL:HG23	2.19	0.43
1:B:355:ASP:OD2	1:B:398:ARG:HD3	2.19	0.43
1:B:835:PRO:HB2	1:B:836:ALA:H	1.62	0.43
1:D:34:HIS:HD2	1:D:38:THR:OG1	2.01	0.43
1:D:396:LEU:HB3	1:D:399:HIS:HB2	2.00	0.43
1:B:63:LEU:HD13	1:B:229:PRO:HG2	2.00	0.43
1:C:676:THR:CG2	1:C:680:LLP:H4'1	2.48	0.43
1:A:19:ALA:HB1	1:A:30:ASN:HD21	1.84	0.43
1:A:381:PRO:O	1:A:386:ARG:NH2	2.52	0.43
1:D:136:LEU:HD22	1:D:338:ASN:ND2	2.34	0.43
1:D:578:LEU:HB3	1:D:666:ILE:HD12	2.01	0.43
1:B:267:LEU:H	1:B:267:LEU:HG	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:NH2	1:B:473:GLU:OE1	2.52	0.43
1:B:795:ARG:O	1:B:799:ARG:HG3	2.19	0.43
1:C:53:PHE:CE1	1:C:188:PRO:HG3	2.53	0.43
1:D:627:GLY:O	1:D:631:ASN:ND2	2.52	0.43
1:D:645:LEU:HD11	1:D:656:VAL:HG21	2.00	0.43
1:A:836:ALA:HA	1:A:837:PRO:HA	1.89	0.43
1:C:458:ILE:O	1:C:462:ILE:HG23	2.19	0.43
1:C:751:SER:O	1:C:752:PRO:C	2.57	0.43
1:D:309:ARG:HB3	1:D:309:ARG:NH1	2.33	0.43
1:D:329:PHE:HB3	1:D:330:PRO:HD3	2.01	0.43
1:D:589:ARG:C	1:D:591:LYS:N	2.72	0.43
1:D:730:GLU:HG3	1:D:731:TYR:N	2.34	0.43
1:A:359:LEU:HD12	1:A:363:LYS:HG2	2.00	0.42
1:A:423:ASP:O	1:A:426:ARG:NH1	2.49	0.42
1:A:724:ARG:C	1:D:729:GLN:HG2	2.40	0.42
1:A:575:ARG:HH22	1:A:776:ASP:HB2	1.84	0.42
1:B:455:VAL:HG13	1:B:484:ASN:ND2	2.34	0.42
1:B:641:ARG:CG	1:B:641:ARG:NH1	2.65	0.42
1:D:264:GLN:OE1	1:D:264:GLN:HA	2.18	0.42
1:D:373:ALA:HA	1:D:449:SER:HB3	2.01	0.42
1:A:571:HIS:H	1:A:576:GLN:NE2	2.16	0.42
1:B:60:ARG:O	1:B:64:VAL:HG13	2.19	0.42
1:C:309:ARG:HH11	1:C:309:ARG:HB3	1.84	0.42
1:C:422:VAL:O	1:C:425:LEU:HB2	2.18	0.42
1:C:741:ILE:H	1:C:741:ILE:HG12	1.60	0.42
1:B:233:TYR:CZ	1:B:234:ARG:HD3	2.55	0.42
1:B:34:HIS:CE1	1:B:61:ASP:OD2	2.68	0.42
1:D:530:PHE:C	1:D:532:ARG:N	2.72	0.42
1:D:650:VAL:O	1:D:650:VAL:CG1	2.66	0.42
1:D:739:ARG:NH1	1:D:739:ARG:HB2	2.34	0.42
1:B:361:TRP:CZ3	1:B:409:ARG:HD2	2.54	0.42
1:C:759:LYS:O	1:C:763:ASN:HB2	2.19	0.42
1:D:499:LEU:N	1:D:537:VAL:HG11	2.35	0.42
1:D:587:TYR:O	1:D:591:LYS:HB2	2.19	0.42
1:D:597:PHE:O	1:D:792:LYS:NZ	2.38	0.42
1:C:19:ALA:HA	1:C:20:GLY:HA3	1.73	0.42
1:D:741:ILE:O	1:D:745:LEU:HG	2.20	0.42
1:A:81:ARG:HG2	1:A:155:TYR:HE2	1.84	0.42
1:A:12:GLN:HE22	1:B:28:LYS:NZ	2.17	0.42
1:C:515:LEU:HD22	1:C:812:SER:HB2	2.01	0.42
1:D:517:GLN:O	1:D:517:GLN:CG	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:LYS:O	1:D:546:ALA:CB	2.68	0.42
1:A:714:ARG:O	1:A:718:VAL:HG23	2.19	0.42
1:D:517:GLN:O	1:D:517:GLN:HG2	2.19	0.42
1:D:683:LEU:HA	1:D:683:LEU:HD23	1.83	0.42
1:C:689:ILE:HA	1:C:709:PHE:O	2.20	0.42
1:D:483:THR:O	1:D:816:THR:HG23	2.19	0.42
1:D:487:THR:HG23	1:D:490:ARG:HB3	2.01	0.42
1:D:665:GLN:HE21	1:D:678:ASN:HA	1.85	0.42
1:D:738:LEU:HB2	1:D:777:TYR:CE2	2.55	0.42
1:D:791:TYR:CA	1:D:797:TRP:CD1	2.97	0.42
1:A:600:PRO:HA	1:A:639:ARG:O	2.20	0.42
1:B:292:ARG:HH21	1:B:341:HIS:CD2	2.38	0.42
1:B:760:ASP:HA	1:B:763:ASN:HB2	2.01	0.42
1:C:378:THR:O	1:C:459:HIS:HE1	2.01	0.42
1:D:562:LEU:HD23	1:D:563:PHE:N	2.35	0.42
1:A:503:ILE:HG12	1:A:521:LEU:HD21	2.02	0.41
1:C:172:GLY:O	1:C:621:LYS:NZ	2.53	0.41
1:C:293:LEU:HD23	1:C:395:LEU:HD21	2.02	0.41
1:D:511:TYR:O	1:D:514:ASP:C	2.57	0.41
1:D:527:ASP:O	1:D:532:ARG:NH2	2.36	0.41
1:D:515:LEU:HD23	1:D:809:GLY:HA2	2.01	0.41
1:A:37:PHE:CD1	1:B:64:VAL:HG22	2.55	0.41
1:C:325:ASN:C	1:C:327:ASP:N	2.74	0.41
1:C:650:VAL:HA	1:C:680:LLP:H2'1	2.02	0.41
1:D:252:PHE:HD2	1:D:269:ARG:HG2	1.86	0.41
1:D:542:LYS:HE3	1:D:563:PHE:CG	2.55	0.41
1:D:822:ARG:NH1	1:D:828:GLU:OE2	2.51	0.41
1:C:73:HIS:CD2	1:C:834:LEU:HD11	2.55	0.41
1:C:774:PHE:C	1:C:776:ASP:H	2.24	0.41
1:D:803:ARG:O	1:D:807:THR:HG22	2.20	0.41
1:C:626:ILE:O	1:C:630:VAL:HG13	2.20	0.41
1:D:571:HIS:ND1	1:D:573:TYR:HD1	2.18	0.41
1:D:715:VAL:HG12	1:D:715:VAL:O	2.21	0.41
1:D:795:ARG:O	1:D:799:ARG:HG3	2.21	0.41
1:D:143:PHE:CG	1:D:817:ILE:HD11	2.56	0.41
1:A:100:VAL:O	1:A:234:ARG:NH1	2.53	0.41
1:A:467:ILE:H	1:A:467:ILE:HD12	1.85	0.41
1:D:168:GLN:HG3	1:D:175:GLN:HG3	2.03	0.41
1:A:85:LEU:CD2	1:A:303:THR:HG21	2.44	0.41
1:C:124:GLU:CD	1:C:655:LYS:HZ1	2.24	0.41
1:C:64:VAL:CG2	1:D:37:PHE:HD1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:GLN:NE2	1:D:678:ASN:OD1	2.53	0.41
1:A:129:ALA:HB1	1:A:131:LEU:HD22	2.03	0.41
1:A:230:VAL:HG22	1:A:230:VAL:O	2.20	0.41
1:A:807:THR:O	1:A:807:THR:HG23	2.21	0.41
1:B:157:TYR:CE2	1:B:242:ARG:HG2	2.56	0.41
1:C:805:ILE:O	1:C:805:ILE:HG22	2.21	0.41
1:D:55:LEU:O	1:D:59:VAL:HG23	2.21	0.41
1:A:136:LEU:HD11	1:A:338:ASN:ND2	2.35	0.41
1:A:495:CYS:HB3	1:A:654:GLU:HB2	2.01	0.41
1:B:67:TRP:HA	1:B:238:VAL:HB	2.03	0.41
1:B:262:TYR:HB3	1:B:264:GLN:HE22	1.85	0.41
1:B:819:GLN:O	1:B:823:GLU:HB2	2.21	0.41
1:C:100:VAL:O	1:C:234:ARG:NH1	2.53	0.41
1:D:764:MET:HE2	3:D:910:HOH:O	2.21	0.41
1:C:727:ASN:O	1:C:730:GLU:HG2	2.21	0.41
1:D:791:TYR:HD1	1:D:797:TRP:CE2	2.38	0.41
1:C:433:GLU:HA	1:C:433:GLU:OE1	2.21	0.41
1:D:235:ASN:OD1	1:D:237:VAL:HG13	2.21	0.41
1:D:363:LYS:HD2	1:D:363:LYS:HA	1.89	0.41
1:A:268:ASP:N	1:A:268:ASP:OD1	2.54	0.40
1:A:34:HIS:CD2	1:A:38:THR:OG1	2.73	0.40
1:B:292:ARG:O	1:B:296:GLU:HG3	2.20	0.40
1:B:571:HIS:H	1:B:576:GLN:NE2	2.18	0.40
1:C:348:GLU:OE1	1:C:399:HIS:HE1	2.04	0.40
1:D:161:TYR:CZ	1:D:279:LEU:HG	2.55	0.40
1:B:571:HIS:O	1:B:576:GLN:NE2	2.54	0.40
1:B:591:LYS:HD3	1:B:591:LYS:HA	1.86	0.40
1:B:170:ILE:HG12	1:B:646:GLU:HG3	2.03	0.40
1:B:458:ILE:HD11	1:B:694:GLY:CA	2.51	0.40
1:C:21:VAL:HG23	1:C:62:HIS:CD2	2.56	0.40
1:C:545:PHE:O	1:C:549:LEU:HB2	2.21	0.40
1:C:717:ASP:OD1	1:C:717:ASP:N	2.54	0.40
1:C:336:GLN:HG3	1:C:825:TRP:HZ2	1.86	0.40
1:C:85:LEU:HD11	1:C:303:THR:HG21	2.02	0.40
1:D:274:ASN:HA	1:D:277:ARG:HB2	2.02	0.40
1:D:36:HIS:O	1:D:40:VAL:HA	2.20	0.40
1:A:766:MET:HA	1:A:766:MET:CE	2.51	0.40
1:D:211:GLN:HG3	1:D:358:ARG:HH22	1.84	0.40
1:D:808:SER:O	1:D:811:PHE:N	2.48	0.40
1:A:515:LEU:HD23	1:A:809:GLY:HA2	2.03	0.40
1:C:53:PHE:CD1	1:C:188:PRO:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:LYS:O	1:C:785:GLU:HB2	2.21	0.40
1:D:665:GLN:NE2	1:D:678:ASN:HA	2.35	0.40
1:A:250:ASN:HB3	1:A:252:PHE:CE2	2.49	0.40
1:A:269:ARG:HH21	1:B:277:ARG:NH2	2.12	0.40
1:A:305:GLN:O	1:A:309:ARG:HB2	2.21	0.40
1:A:682:MET:HE3	1:A:808:SER:CB	2.39	0.40
1:C:347:PRO:HD3	1:C:444:LEU:HD11	2.03	0.40
1:D:399:HIS:O	1:D:403:ILE:HG13	2.22	0.40
1:D:433:GLU:HG2	1:D:433:GLU:H	1.72	0.40
1:D:523:SER:HB2	1:D:524:TYR:CE1	2.56	0.40
1:D:571:HIS:CD2	1:D:613:TYR:CE2	3.09	0.40
1:D:584:ILE:HD11	1:D:626:ILE:HD11	2.03	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	801/842 (95%)	745 (93%)	43 (5%)	13 (2%)	11	23
1	B	802/842 (95%)	754 (94%)	37 (5%)	11 (1%)	13	26
1	C	798/842 (95%)	746 (94%)	43 (5%)	9 (1%)	17	35
1	D	797/842 (95%)	698 (88%)	78 (10%)	21 (3%)	6	10
All	All	3198/3368 (95%)	2943 (92%)	201 (6%)	54 (2%)	11	21

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	514	ASP
1	A	551	ARG

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Mol	Chain	Res	Type
1	A	835	PRO
1	B	678	ASN
1	B	835	PRO
1	C	16	ARG
1	C	19	ALA
1	C	166	PHE
1	C	325	ASN
1	D	21	VAL
1	D	509	GLU
1	D	510	GLU
1	D	590	ILE
1	D	801	VAL
1	A	166	PHE
1	A	261	GLY
1	A	421	ASP
1	A	477	HIS
1	C	18	LEU
1	C	724	ARG
1	D	166	PHE
1	D	489	ARG
1	D	724	ARG
1	D	792	LYS
1	A	473	GLU
1	B	166	PHE
1	B	211	GLN
1	B	613	TYR
1	D	576	GLN
1	D	591	LYS
1	D	596	LYS
1	D	693	ASP
1	A	836	ALA
1	B	421	ASP
1	C	778	GLU
1	D	251	ASP
1	D	540	GLU
1	D	561	SER
1	D	697	VAL
1	A	329	PHE
1	B	268	ASP
1	B	551	ARG
1	C	752	PRO
1	D	830	SER

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Mol	Chain	Res	Type
1	B	836	ALA
1	C	775	ALA
1	D	523	SER
1	D	558	ASN
1	A	260	GLY
1	B	20	GLY
1	D	836	ALA
1	A	263	ILE
1	B	837	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	699/730 (96%)	604 (86%)	95 (14%)	4	7
1	B	700/730 (96%)	609 (87%)	91 (13%)	5	8
1	C	697/730 (96%)	626 (90%)	71 (10%)	8	16
1	D	697/730 (96%)	593 (85%)	104 (15%)	3	6
All	All	2793/2920 (96%)	2432 (87%)	361 (13%)	5	9

All (361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	10	ARG
1	A	15	VAL
1	A	16	ARG
1	A	18	LEU
1	A	23	ASN
1	A	29	LYS
1	A	39	LEU
1	A	63	LEU
1	A	71	GLN
1	A	76	GLU
1	A	81	ARG

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Mol	Chain	Res	Type
1	A	82	ILE
1	A	90	TYR
1	A	91	MET
1	A	95	LEU
1	A	128	ASP
1	A	131	LEU
1	A	138	ARG
1	A	169	LYS
1	A	216	VAL
1	A	228	THR
1	A	230	VAL
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	243	LEU
1	A	251	ASP
1	A	262	TYR
1	A	264	GLN
1	A	268	ASP
1	A	274	ASN
1	A	287	GLU
1	A	292	ARG
1	A	325	ASN
1	A	332	LYS
1	A	339	ASP
1	A	358	ARG
1	A	361	TRP
1	A	371	THR
1	A	380	LEU
1	A	382	GLU
1	A	391	LEU
1	A	392	LEU
1	A	396	LEU
1	A	400	LEU
1	A	408	GLN
1	A	425	LEU
1	A	426	ARG
1	A	437	LYS
1	A	438	ARG
1	A	441	MET
1	A	444	LEU
1	A	449	SER

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Mol	Chain	Res	Type
1	A	453	ASN
1	A	455	VAL
1	A	457	ARG
1	A	458	ILE
1	A	486	ILE
1	A	490	ARG
1	A	492	LEU
1	A	521	LEU
1	A	522	LEU
1	A	543	LEU
1	A	549	LEU
1	A	554	LYS
1	A	565	VAL
1	A	568	LYS
1	A	569	ARG
1	A	576	GLN
1	A	579	ASN
1	A	593	GLU
1	A	622	LEU
1	A	639	ARG
1	A	640	LEU
1	A	649	ARG
1	A	652	LEU
1	A	662	LEU
1	A	678	ASN
1	A	683	LEU
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	713	MET
1	A	714	ARG
1	A	716	GLU
1	A	743	GLU
1	A	749	PHE
1	A	753	LYS
1	A	760	ASP
1	A	765	LEU
1	A	782	LYS
1	A	797	TRP
1	A	807	THR
1	A	827	VAL
1	B	10	ARG

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Mol	Chain	Res	Type
1	B	15	VAL
1	B	21	VAL
1	B	39	LEU
1	B	64	VAL
1	B	66	ARG
1	B	69	ARG
1	B	82	ILE
1	B	85	LEU
1	B	90	TYR
1	B	91	MET
1	B	94	THR
1	B	95	LEU
1	B	100	VAL
1	B	104	LEU
1	B	128	ASP
1	B	131	LEU
1	B	138	ARG
1	B	165	ILE
1	B	171	CYS
1	B	177	GLU
1	B	191	LYS
1	B	214	LYS
1	B	234	ARG
1	B	235	ASN
1	B	242	ARG
1	B	251	ASP
1	B	262	TYR
1	B	264	GLN
1	B	267	LEU
1	B	269	ARG
1	B	274	ASN
1	B	289	LYS
1	B	291	LEU
1	B	314	SER
1	B	325	ASN
1	B	337	LEU
1	B	339	ASP
1	B	359	LEU
1	B	360	ASP
1	B	361	TRP
1	B	363	LYS
1	B	380	LEU

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Mol	Chain	Res	Type
1	B	382	GLU
1	B	392	LEU
1	B	396	LEU
1	B	400	LEU
1	B	423	ASP
1	B	425	LEU
1	B	444	LEU
1	B	462	ILE
1	B	469	LYS
1	B	474	LEU
1	B	486	ILE
1	B	489	ARG
1	B	492	LEU
1	B	506	ARG
1	B	516	ASP
1	B	525	VAL
1	B	554	LYS
1	B	560	ASN
1	B	569	ARG
1	B	574	LYS
1	B	576	GLN
1	B	579	ASN
1	B	589	ARG
1	B	613	TYR
1	B	622	LEU
1	B	640	LEU
1	B	641	ARG
1	B	649	ARG
1	B	652	LEU
1	B	662	LEU
1	B	665	GLN
1	B	667	SER
1	B	676	THR
1	B	683	LEU
1	B	692	MET
1	B	706	GLU
1	B	708	PHE
1	B	714	ARG
1	B	737	GLU
1	B	741	ILE
1	B	745	LEU
1	B	753	LYS

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Mol	Chain	Res	Type
1	B	765	LEU
1	B	766	MET
1	B	768	HIS
1	B	779	GLU
1	B	833	ARG
1	B	839	GLU
1	C	9	LYS
1	C	12	GLN
1	C	15	VAL
1	C	16	ARG
1	C	18	LEU
1	C	23	ASN
1	C	39	LEU
1	C	64	VAL
1	C	66	ARG
1	C	90	TYR
1	C	95	LEU
1	C	128	ASP
1	C	131	LEU
1	C	169	LYS
1	C	177	GLU
1	C	191	LYS
1	C	195	GLU
1	C	234	ARG
1	C	235	ASN
1	C	237	VAL
1	C	242	ARG
1	C	243	LEU
1	C	247	LYS
1	C	254	LEU
1	C	264	GLN
1	C	267	LEU
1	C	274	ASN
1	C	278	VAL
1	C	279	LEU
1	C	292	ARG
1	C	332	LYS
1	C	337	LEU
1	C	339	ASP
1	C	356	LEU
1	C	361	TRP
1	C	378	THR

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Mol	Chain	Res	Type
1	C	384	LEU
1	C	395	LEU
1	C	396	LEU
1	C	400	LEU
1	C	425	LEU
1	C	474	LEU
1	C	486	ILE
1	C	492	LEU
1	C	509	GLU
1	C	522	LEU
1	C	538	LYS
1	C	539	GLN
1	C	543	LEU
1	C	565	VAL
1	C	576	GLN
1	C	579	ASN
1	C	584	ILE
1	C	622	LEU
1	C	630	VAL
1	C	639	ARG
1	C	641	ARG
1	C	652	LEU
1	C	662	LEU
1	C	676	THR
1	C	678	ASN
1	C	683	LEU
1	C	714	ARG
1	C	717	ASP
1	C	724	ARG
1	C	741	ILE
1	C	753	LYS
1	C	760	ASP
1	C	763	ASN
1	C	788	SER
1	C	833	ARG
1	D	15	VAL
1	D	16	ARG
1	D	21	VAL
1	D	39	LEU
1	D	47	THR
1	D	64	VAL
1	D	77	LYS

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Mol	Chain	Res	Type
1	D	81	ARG
1	D	82	ILE
1	D	85	LEU
1	D	87	LEU
1	D	88	GLU
1	D	90	TYR
1	D	91	MET
1	D	95	LEU
1	D	100	VAL
1	D	128	ASP
1	D	131	LEU
1	D	136	LEU
1	D	138	ARG
1	D	171	CYS
1	D	191	LYS
1	D	211	GLN
1	D	237	VAL
1	D	242	ARG
1	D	245	SER
1	D	247	LYS
1	D	264	GLN
1	D	269	ARG
1	D	274	ASN
1	D	280	TYR
1	D	292	ARG
1	D	304	LEU
1	D	310	ARG
1	D	332	LYS
1	D	337	LEU
1	D	358	ARG
1	D	361	TRP
1	D	382	GLU
1	D	392	LEU
1	D	396	LEU
1	D	400	LEU
1	D	405	GLU
1	D	425	LEU
1	D	426	ARG
1	D	433	GLU
1	D	437	LYS
1	D	444	LEU
1	D	457	ARG

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Mol	Chain	Res	Type
1	D	469	LYS
1	D	474	LEU
1	D	486	ILE
1	D	489	ARG
1	D	490	ARG
1	D	492	LEU
1	D	501	GLU
1	D	517	GLN
1	D	518	LEU
1	D	522	LEU
1	D	526	ASP
1	D	528	GLU
1	D	530	PHE
1	D	532	ARG
1	D	536	LYS
1	D	555	VAL
1	D	561	SER
1	D	576	GLN
1	D	579	ASN
1	D	583	VAL
1	D	585	THR
1	D	617	LYS
1	D	622	LEU
1	D	629	VAL
1	D	649	ARG
1	D	652	LEU
1	D	665	GLN
1	D	667	SER
1	D	676	THR
1	D	679	MET
1	D	683	LEU
1	D	688	THR
1	D	702	GLU
1	D	705	GLU
1	D	706	GLU
1	D	713	MET
1	D	716	GLU
1	D	723	GLN
1	D	724	ARG
1	D	727	ASN
1	D	735	ILE
1	D	746	SER

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Mol	Chain	Res	Type
1	D	753	LYS
1	D	756	ASP
1	D	759	LYS
1	D	765	LEU
1	D	766	MET
1	D	770	ARG
1	D	782	LYS
1	D	795	ARG
1	D	810	LYS
1	D	812	SER
1	D	813	SER
1	D	823	GLU
1	D	827	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	ASN
1	A	30	ASN
1	A	34	HIS
1	A	114	GLN
1	A	167	ASN
1	A	168	GLN
1	A	235	ASN
1	A	264	GLN
1	A	274	ASN
1	A	325	ASN
1	A	336	GLN
1	A	399	HIS
1	A	408	GLN
1	A	412	ASN
1	A	459	HIS
1	A	481	ASN
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	582	HIS
1	A	727	ASN
1	A	744	GLN
1	A	754	GLN

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Mol	Chain	Res	Type
1	B	12	GLN
1	B	34	HIS
1	B	44	ASN
1	B	167	ASN
1	B	168	GLN
1	B	211	GLN
1	B	235	ASN
1	B	264	GLN
1	B	274	ASN
1	B	325	ASN
1	B	336	GLN
1	B	377	HIS
1	B	399	HIS
1	B	453	ASN
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	696	ASN
1	B	727	ASN
1	B	744	GLN
1	C	23	ASN
1	C	34	HIS
1	C	168	GLN
1	C	235	ASN
1	C	274	ASN
1	C	336	GLN
1	C	399	HIS
1	C	412	ASN
1	C	453	ASN
1	C	459	HIS
1	C	481	ASN
1	C	541	ASN
1	C	566	GLN
1	C	576	GLN
1	C	579	ASN
1	C	727	ASN
1	C	744	GLN
1	C	763	ASN
1	C	768	HIS

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Mol	Chain	Res	Type
1	D	34	HIS
1	D	44	ASN
1	D	73	HIS
1	D	168	GLN
1	D	187	ASN
1	D	274	ASN
1	D	336	GLN
1	D	338	ASN
1	D	341	HIS
1	D	377	HIS
1	D	399	HIS
1	D	459	HIS
1	D	481	ASN
1	D	541	ASN
1	D	566	GLN
1	D	576	GLN
1	D	579	ASN
1	D	696	ASN
1	D	723	GLN
1	D	727	ASN
1	D	744	GLN
1	D	767	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	A	680	1	24,24,25	1.84	6 (25%)	28,32,34	1.26	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	B	680	1	24,24,25	1.83	6 (25%)	28,32,34	1.25	4 (14%)
1	LLP	C	680	1	24,24,25	1.78	5 (20%)	28,32,34	1.25	3 (10%)
1	LLP	D	680	1	24,24,25	1.78	5 (20%)	28,32,34	1.38	5 (17%)

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
1	LLP	A	680	1	-	0/15/17/19	0/1/1/1
1	LLP	B	680	1	-	0/15/17/19	0/1/1/1
1	LLP	C	680	1	-	0/15/17/19	0/1/1/1
1	LLP	D	680	1	-	0/15/17/19	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O3-C3	-6.30	1.22	1.37
1	D	680	LLP	O3-C3	-5.96	1.23	1.37
1	B	680	LLP	O3-C3	-5.89	1.23	1.37
1	C	680	LLP	O3-C3	-5.79	1.23	1.37
1	A	680	LLP	C3-C2	-2.00	1.39	1.40
1	A	680	LLP	C2-N1	2.06	1.38	1.33
1	B	680	LLP	C6-N1	2.10	1.38	1.34
1	B	680	LLP	C2-N1	2.23	1.38	1.33
1	D	680	LLP	C2-N1	2.27	1.38	1.33
1	C	680	LLP	C2-N1	2.32	1.38	1.33
1	D	680	LLP	C4'-NZ	2.40	1.34	1.27
1	C	680	LLP	C4'-NZ	2.42	1.34	1.27
1	B	680	LLP	C4'-NZ	2.42	1.34	1.27
1	A	680	LLP	CE-NZ	2.42	1.51	1.46
1	A	680	LLP	C4'-NZ	2.56	1.34	1.27
1	D	680	LLP	CE-NZ	2.58	1.52	1.46
1	C	680	LLP	C4-C4'	2.63	1.51	1.46
1	B	680	LLP	C4-C4'	2.66	1.51	1.46
1	C	680	LLP	CA-C	2.66	1.53	1.50
1	A	680	LLP	C4-C4'	2.85	1.51	1.46
1	B	680	LLP	CA-C	2.87	1.54	1.50
1	D	680	LLP	C4-C4'	3.15	1.52	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C4-C4'-NZ	-2.77	111.22	124.66
1	A	680	LLP	C5-C6-N1	-2.76	119.20	123.87
1	D	680	LLP	CE-NZ-C4'	-2.63	111.39	119.03
1	B	680	LLP	C4-C4'-NZ	-2.57	112.19	124.66
1	C	680	LLP	CE-NZ-C4'	-2.56	111.60	119.03
1	C	680	LLP	C5-C6-N1	-2.41	119.79	123.87
1	D	680	LLP	C5'-C5-C6	-2.34	115.31	119.33
1	C	680	LLP	C4-C4'-NZ	-2.34	113.31	124.66
1	D	680	LLP	C5-C6-N1	-2.31	119.96	123.87
1	B	680	LLP	C5-C6-N1	-2.27	120.03	123.87
1	A	680	LLP	OP3-P-OP4	-2.25	100.74	106.73
1	B	680	LLP	CE-NZ-C4'	-2.16	112.77	119.03
1	D	680	LLP	OP4-C5'-C5	-2.07	105.15	109.32
1	A	680	LLP	CE-NZ-C4'	-2.03	113.14	119.03
1	D	680	LLP	CD-CE-NZ	2.36	116.10	110.88
1	B	680	LLP	OP4-C5'-C5	2.66	114.67	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	680	LLP	3	0
1	B	680	LLP	2	0
1	C	680	LLP	7	0
1	D	680	LLP	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	SO4	A	900	-	4,4,4	0.15	0	6,6,6	0.35	0
2	SO4	A	901	-	4,4,4	0.24	0	6,6,6	0.40	0
2	SO4	A	902	-	4,4,4	0.17	0	6,6,6	0.41	0
2	SO4	B	900	-	4,4,4	0.24	0	6,6,6	0.19	0
2	SO4	B	901	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	B	902	-	4,4,4	0.19	0	6,6,6	0.38	0
2	SO4	C	901	-	4,4,4	0.25	0	6,6,6	0.55	0
2	SO4	C	902	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	D	900	-	4,4,4	0.23	0	6,6,6	0.36	0
2	SO4	D	901	-	4,4,4	0.25	0	6,6,6	0.26	0
2	SO4	D	902	-	4,4,4	0.23	0	6,6,6	0.28	0
2	SO4	D	903	-	4,4,4	0.12	0	6,6,6	0.27	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	SO4	A	900	-	-	0/0/0/0	0/0/0/0
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
2	SO4	B	900	-	-	0/0/0/0	0/0/0/0
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	SO4	B	902	-	-	0/0/0/0	0/0/0/0
2	SO4	C	901	-	-	0/0/0/0	0/0/0/0
2	SO4	C	902	-	-	0/0/0/0	0/0/0/0
2	SO4	D	900	-	-	0/0/0/0	0/0/0/0
2	SO4	D	901	-	-	0/0/0/0	0/0/0/0
2	SO4	D	902	-	-	0/0/0/0	0/0/0/0
2	SO4	D	903	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	SO4	1	0
2	D	900	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	809/842 (96%)	0.18	35 (4%)	36	28	29, 46, 62, 74	0
1	B	810/842 (96%)	0.17	35 (4%)	36	28	28, 46, 66, 78	0
1	C	806/842 (95%)	0.22	37 (4%)	33	26	23, 48, 71, 83	0
1	D	805/842 (95%)	0.42	62 (7%)	14	10	34, 53, 87, 102	0
All	All	3230/3368 (95%)	0.25	169 (5%)	28	21	23, 48, 73, 102	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	GLY	7.8
1	A	252	PHE	6.6
1	D	252	PHE	6.4
1	C	252	PHE	6.1
1	A	260	GLY	6.0
1	A	75	TYR	5.4
1	D	530	PHE	5.3
1	A	261	GLY	5.3
1	B	288	GLY	5.3
1	C	324	THR	5.2
1	C	253	ASN	4.7
1	C	254	LEU	4.7
1	D	597	PHE	4.6
1	B	252	PHE	4.5
1	A	281	PRO	4.4
1	D	22	GLU	4.2
1	A	165	ILE	4.2
1	D	543	LEU	4.0
1	B	314	SER	3.9
1	D	789	ALA	3.9
1	C	556	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	833	ARG	3.9
1	B	553	TYR	3.8
1	D	113	TYR	3.8
1	B	554	LYS	3.8
1	B	165	ILE	3.8
1	C	580	CYS	3.8
1	C	565	VAL	3.7
1	D	598	VAL	3.6
1	B	176	MET	3.5
1	B	551	ARG	3.5
1	B	280	TYR	3.5
1	C	251	ASP	3.5
1	D	527	ASP	3.5
1	B	345	ALA	3.5
1	A	418	PHE	3.4
1	C	598	VAL	3.4
1	C	597	PHE	3.3
1	D	632	HIS	3.3
1	D	556	HIS	3.3
1	D	733	ASP	3.3
1	A	422	VAL	3.3
1	A	612	GLY	3.2
1	B	21	VAL	3.2
1	B	720	ARG	3.2
1	B	251	ASP	3.2
1	D	250	ASN	3.2
1	D	75	TYR	3.2
1	D	522	LEU	3.2
1	A	380	LEU	3.2
1	D	210	SER	3.1
1	B	337	LEU	3.1
1	D	507	ILE	3.0
1	C	525	VAL	3.0
1	D	536	LYS	3.0
1	D	287	GLU	3.0
1	D	509	GLU	2.9
1	A	16	ARG	2.9
1	B	380	LEU	2.9
1	C	579	ASN	2.9
1	C	526	ASP	2.9
1	D	777	TYR	2.9
1	D	85	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	791	TYR	2.9
1	C	16	ARG	2.8
1	A	210	SER	2.8
1	B	723	GLN	2.8
1	C	835	PRO	2.8
1	A	426	ARG	2.8
1	B	344	LEU	2.8
1	A	211	GLN	2.7
1	D	595	ASN	2.7
1	D	211	GLN	2.7
1	D	692	MET	2.7
1	D	715	VAL	2.7
1	C	768	HIS	2.7
1	C	752	PRO	2.7
1	A	337	LEU	2.6
1	A	372	CYS	2.6
1	A	565	VAL	2.6
1	A	723	GLN	2.6
1	D	553	TYR	2.6
1	D	561	SER	2.6
1	D	164	GLY	2.6
1	D	594	PRO	2.6
1	A	554	LYS	2.6
1	D	592	LYS	2.6
1	A	10	ARG	2.6
1	D	630	VAL	2.6
1	C	262	TYR	2.6
1	C	553	TYR	2.6
1	B	838	ASP	2.6
1	C	10	ARG	2.6
1	C	263	ILE	2.5
1	D	533	ASP	2.5
1	C	250	ASN	2.5
1	D	251	ASP	2.5
1	B	382	GLU	2.5
1	C	581	LEU	2.5
1	D	10	ARG	2.5
1	A	676	THR	2.5
1	C	554	LYS	2.5
1	B	271	LEU	2.5
1	C	113	TYR	2.5
1	C	753	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	280	TYR	2.4
1	A	342	PRO	2.4
1	D	634	PRO	2.4
1	C	345	ALA	2.4
1	B	75	TYR	2.4
1	B	833	ARG	2.4
1	D	726	TYR	2.4
1	A	287	GLU	2.4
1	C	833	ARG	2.4
1	D	314	SER	2.4
1	D	635	VAL	2.4
1	A	580	CYS	2.4
1	D	728	ALA	2.3
1	B	343	SER	2.3
1	D	531	ILE	2.3
1	A	415	ALA	2.3
1	B	211	GLN	2.3
1	C	792	LYS	2.3
1	A	259	VAL	2.3
1	A	382	GLU	2.3
1	C	720	ARG	2.3
1	A	381	PRO	2.3
1	C	560	ASN	2.3
1	D	324	THR	2.3
1	A	22	GLU	2.3
1	D	795	ARG	2.2
1	D	525	VAL	2.2
1	B	580	CYS	2.2
1	D	545	PHE	2.2
1	B	565	VAL	2.2
1	C	548	TYR	2.2
1	B	445	CYS	2.2
1	D	165	ILE	2.2
1	B	113	TYR	2.2
1	D	379	VAL	2.2
1	D	534	VAL	2.2
1	A	288	GLY	2.2
1	B	20	GLY	2.2
1	B	16	ARG	2.1
1	C	749	PHE	2.1
1	D	600	PRO	2.1
1	B	552	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	837	PRO	2.1
1	B	548	TYR	2.1
1	B	163	PHE	2.1
1	B	792	LYS	2.1
1	D	560	ASN	2.1
1	A	472	TYR	2.1
1	D	557	ILE	2.1
1	C	551	ARG	2.1
1	B	576	GLN	2.1
1	D	465	LYS	2.1
1	D	709	PHE	2.1
1	D	782	LYS	2.1
1	C	718	VAL	2.0
1	D	420	GLY	2.0
1	D	695	ALA	2.0
1	A	768	HIS	2.0
1	C	208	HIS	2.0
1	D	169	LYS	2.0
1	D	209	THR	2.0
1	D	555	VAL	2.0
1	A	85	LEU	2.0
1	C	280	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	D	680	24/25	0.94	0.15	-	51,58,62,63	0
1	LLP	C	680	24/25	0.97	0.15	-	40,42,48,49	0
1	LLP	B	680	24/25	0.97	0.18	-	37,38,40,42	0
1	LLP	A	680	24/25	0.96	0.19	-	28,31,36,39	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	901	5/5	0.86	0.23	3.18	74,76,77,77	0
2	SO4	A	901	5/5	0.86	0.19	1.52	82,83,83,84	0
2	SO4	B	901	5/5	0.91	0.19	0.87	76,77,79,79	0
2	SO4	B	900	5/5	0.92	0.23	0.34	81,81,82,83	0
2	SO4	D	900	5/5	0.83	0.22	0.16	88,89,89,90	0
2	SO4	A	902	5/5	0.90	0.16	-0.50	79,80,81,81	0
2	SO4	D	901	5/5	0.93	0.17	-0.61	83,84,84,85	0
2	SO4	B	902	5/5	0.97	0.12	-0.78	58,58,58,60	0
2	SO4	D	903	5/5	0.94	0.14	-0.87	68,69,69,70	0
2	SO4	A	900	5/5	0.95	0.14	-1.03	71,72,72,73	0
2	SO4	C	902	5/5	0.98	0.09	-3.90	64,64,65,65	0
2	SO4	D	902	5/5	0.93	0.15	-	77,77,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.