



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:06 AM GMT

PDB ID : 3O3C
Title : Glycogen synthase basal state UDP complex
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2010-07-23
Resolution : 3.51 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

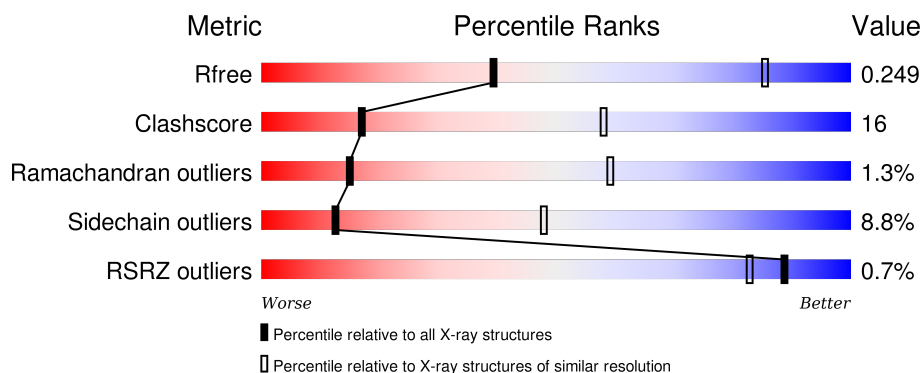
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	725	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	725	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>27%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	725	<div> <div></div> <div> <div>54%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	725	<div> <div></div> <div> <div>55%</div> <div>25%</div> <div>•</div> <div>16%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	802	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19847 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 [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	B	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	C	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	D	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P27472
A	-18	GLY	-	EXPRESSION TAG	UNP P27472
A	-17	SER	-	EXPRESSION TAG	UNP P27472
A	-16	SER	-	EXPRESSION TAG	UNP P27472
A	-15	HIS	-	EXPRESSION TAG	UNP P27472
A	-14	HIS	-	EXPRESSION TAG	UNP P27472
A	-13	HIS	-	EXPRESSION TAG	UNP P27472
A	-12	HIS	-	EXPRESSION TAG	UNP P27472
A	-11	HIS	-	EXPRESSION TAG	UNP P27472
A	-10	HIS	-	EXPRESSION TAG	UNP P27472
A	-9	SER	-	EXPRESSION TAG	UNP P27472
A	-8	SER	-	EXPRESSION TAG	UNP P27472
A	-7	GLY	-	EXPRESSION TAG	UNP P27472
A	-6	LEU	-	EXPRESSION TAG	UNP P27472
A	-5	VAL	-	EXPRESSION TAG	UNP P27472
A	-4	PRO	-	EXPRESSION TAG	UNP P27472
A	-3	ARG	-	EXPRESSION TAG	UNP P27472
A	-2	GLY	-	EXPRESSION TAG	UNP P27472
A	-1	SER	-	EXPRESSION TAG	UNP P27472
A	0	HIS	-	EXPRESSION TAG	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	EXPRESSION TAG	UNP P27472
B	-14	HIS	-	EXPRESSION TAG	UNP P27472
B	-13	HIS	-	EXPRESSION TAG	UNP P27472
B	-12	HIS	-	EXPRESSION TAG	UNP P27472
B	-11	HIS	-	EXPRESSION TAG	UNP P27472
B	-10	HIS	-	EXPRESSION TAG	UNP P27472
B	-9	SER	-	EXPRESSION TAG	UNP P27472
B	-8	SER	-	EXPRESSION TAG	UNP P27472
B	-7	GLY	-	EXPRESSION TAG	UNP P27472
B	-6	LEU	-	EXPRESSION TAG	UNP P27472
B	-5	VAL	-	EXPRESSION TAG	UNP P27472
B	-4	PRO	-	EXPRESSION TAG	UNP P27472
B	-3	ARG	-	EXPRESSION TAG	UNP P27472
B	-2	GLY	-	EXPRESSION TAG	UNP P27472
B	-1	SER	-	EXPRESSION TAG	UNP P27472
B	0	HIS	-	EXPRESSION TAG	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	-19	MET	-	EXPRESSION TAG	UNP P27472
C	-18	GLY	-	EXPRESSION TAG	UNP P27472
C	-17	SER	-	EXPRESSION TAG	UNP P27472
C	-16	SER	-	EXPRESSION TAG	UNP P27472
C	-15	HIS	-	EXPRESSION TAG	UNP P27472
C	-14	HIS	-	EXPRESSION TAG	UNP P27472
C	-13	HIS	-	EXPRESSION TAG	UNP P27472
C	-12	HIS	-	EXPRESSION TAG	UNP P27472
C	-11	HIS	-	EXPRESSION TAG	UNP P27472
C	-10	HIS	-	EXPRESSION TAG	UNP P27472
C	-9	SER	-	EXPRESSION TAG	UNP P27472
C	-8	SER	-	EXPRESSION TAG	UNP P27472
C	-7	GLY	-	EXPRESSION TAG	UNP P27472
C	-6	LEU	-	EXPRESSION TAG	UNP P27472
C	-5	VAL	-	EXPRESSION TAG	UNP P27472

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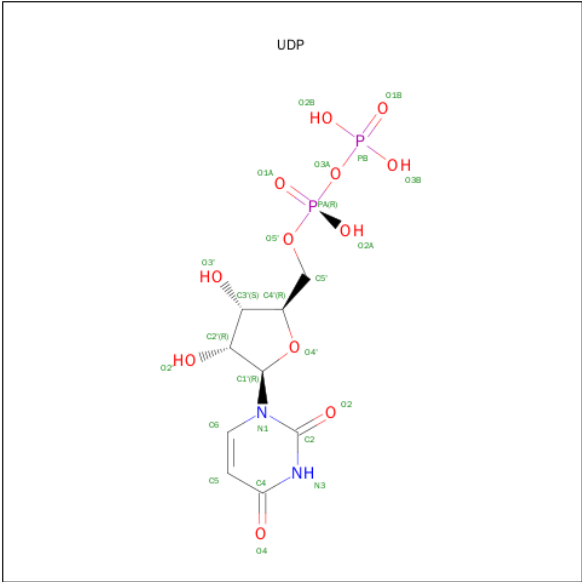
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP P27472
C	-3	ARG	-	EXPRESSION TAG	UNP P27472
C	-2	GLY	-	EXPRESSION TAG	UNP P27472
C	-1	SER	-	EXPRESSION TAG	UNP P27472
C	0	HIS	-	EXPRESSION TAG	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	-19	MET	-	EXPRESSION TAG	UNP P27472
D	-18	GLY	-	EXPRESSION TAG	UNP P27472
D	-17	SER	-	EXPRESSION TAG	UNP P27472
D	-16	SER	-	EXPRESSION TAG	UNP P27472
D	-15	HIS	-	EXPRESSION TAG	UNP P27472
D	-14	HIS	-	EXPRESSION TAG	UNP P27472
D	-13	HIS	-	EXPRESSION TAG	UNP P27472
D	-12	HIS	-	EXPRESSION TAG	UNP P27472
D	-11	HIS	-	EXPRESSION TAG	UNP P27472
D	-10	HIS	-	EXPRESSION TAG	UNP P27472
D	-9	SER	-	EXPRESSION TAG	UNP P27472
D	-8	SER	-	EXPRESSION TAG	UNP P27472
D	-7	GLY	-	EXPRESSION TAG	UNP P27472
D	-6	LEU	-	EXPRESSION TAG	UNP P27472
D	-5	VAL	-	EXPRESSION TAG	UNP P27472
D	-4	PRO	-	EXPRESSION TAG	UNP P27472
D	-3	ARG	-	EXPRESSION TAG	UNP P27472
D	-2	GLY	-	EXPRESSION TAG	UNP P27472
D	-1	SER	-	EXPRESSION TAG	UNP P27472
D	0	HIS	-	EXPRESSION TAG	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472

- 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	D	1	Total	O	S	0	0
			5	4	1		
2	A	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	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	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 URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).

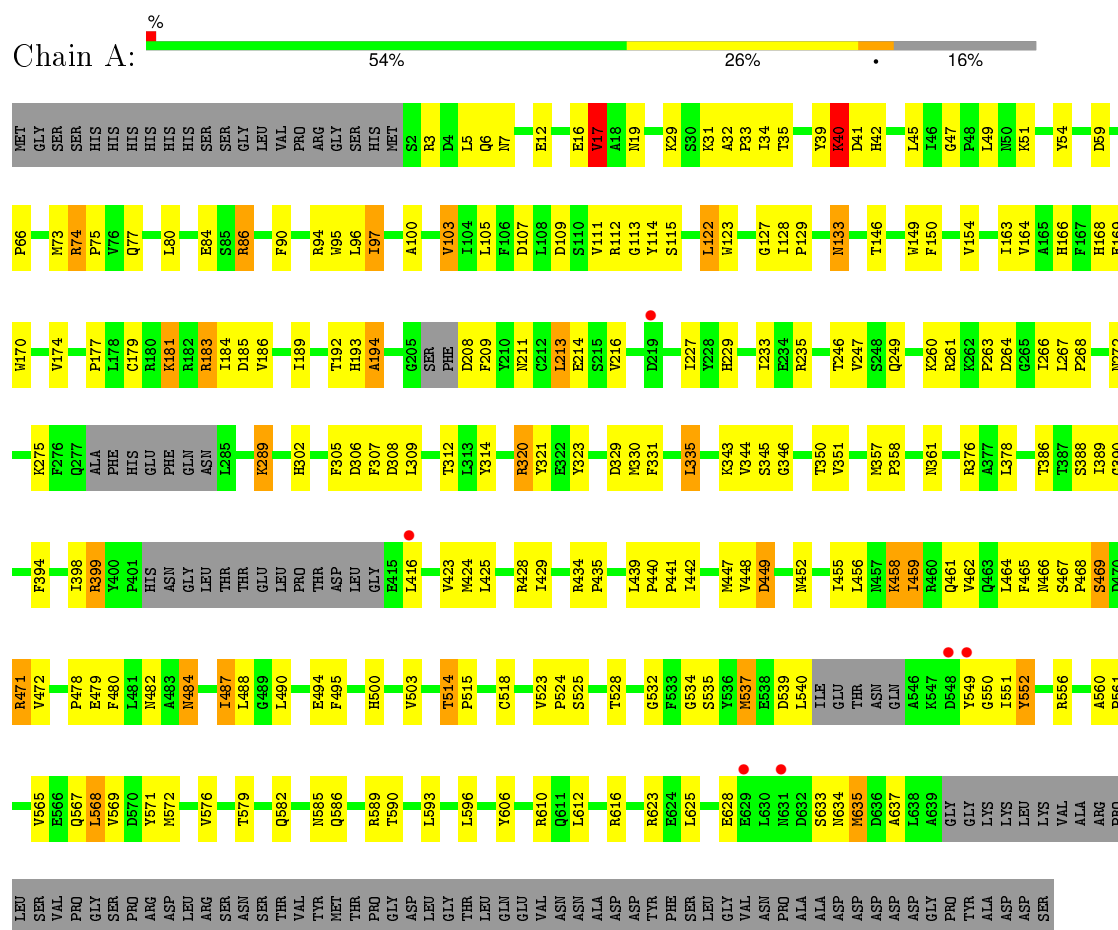


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

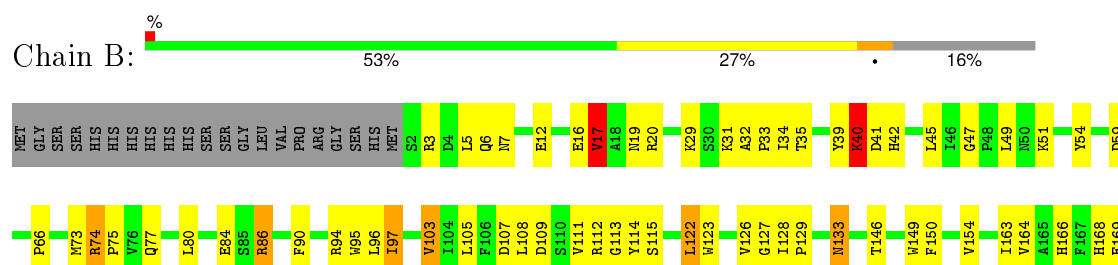
3 Residue-property plots

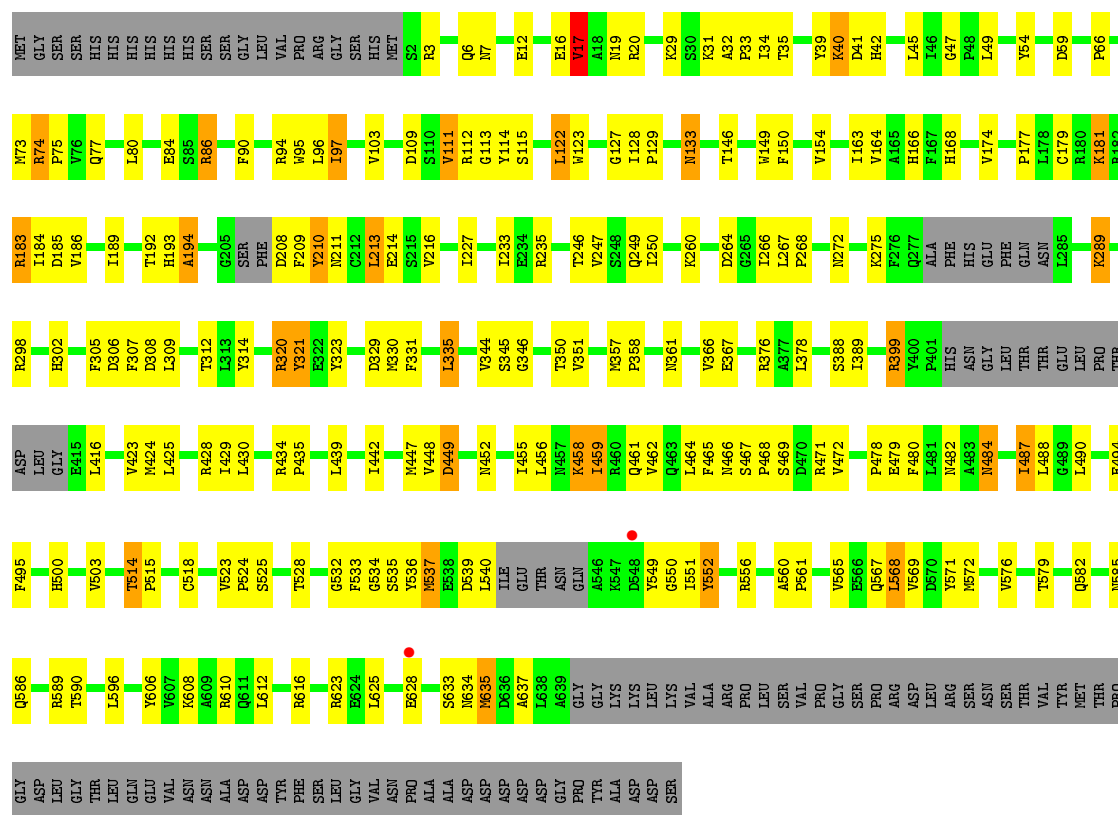
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 [starch] synthase isoform 2



- Molecule 1: Glycogen [starch] synthase isoform 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.59Å 167.21Å 121.25Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	48.29 – 3.51 48.29 – 3.51	Depositor EDS
% Data completeness (in resolution range)	50.2 (48.29-3.51) 98.9 (48.29-3.51)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.219 , 0.249 0.219 , 0.249	Depositor DCC
R_{free} test set	2385 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	104.4	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 85.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46349 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19847	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, 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	0.46	0/5038	0.58	0/6819
1	B	0.45	0/5038	0.58	0/6819
1	C	0.44	0/5038	0.57	1/6819 (0.0%)
1	D	0.45	0/5038	0.57	0/6819
All	All	0.45	0/20152	0.58	1/27276 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LEU	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4923	0	4850	168	0
1	B	4923	0	4850	170	0
1	C	4923	0	4850	158	0
1	D	4923	0	4850	161	0
2	A	10	0	0	0	0
2	B	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	0	0	0
2	D	15	0	0	1	0
3	A	25	0	11	2	0
3	B	25	0	11	2	0
3	C	25	0	11	4	0
3	D	25	0	11	3	0
All	All	19847	0	19444	639	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 16.

All (639) 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:320:ARG:HB2	1:A:320:ARG:HH11	1.19	1.07
1:C:320:ARG:HB2	1:C:320:ARG:HH11	1.23	1.04
1:B:320:ARG:HH11	1:B:320:ARG:HB2	1.20	1.02
1:B:320:ARG:HH11	1:B:320:ARG:CB	1.74	1.01
1:D:320:ARG:HB2	1:D:320:ARG:HH11	1.24	1.01
1:C:29:LYS:HG3	1:C:97:ILE:HG21	1.42	1.01
1:B:29:LYS:HG3	1:B:97:ILE:HG21	1.43	1.00
1:D:29:LYS:HG3	1:D:97:ILE:HG21	1.43	1.00
1:A:320:ARG:CB	1:A:320:ARG:HH11	1.74	0.99
1:A:29:LYS:HG3	1:A:97:ILE:HG21	1.43	0.99
1:C:320:ARG:HH11	1:C:320:ARG:CB	1.77	0.98
1:D:320:ARG:HH11	1:D:320:ARG:CB	1.78	0.96
1:A:390:GLY:HA2	1:C:386:THR:HG21	1.54	0.88
1:A:320:ARG:HB2	1:A:320:ARG:NH1	1.91	0.85
1:B:399:ARG:NH2	1:D:307:PHE:O	2.10	0.85
1:B:320:ARG:HB2	1:B:320:ARG:NH1	1.92	0.84
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.60	0.84
1:B:549:TYR:O	1:B:590:THR:HG22	1.77	0.83
1:A:550:GLY:HA3	1:A:590:THR:HG22	1.61	0.83
1:A:549:TYR:O	1:A:590:THR:HG22	1.77	0.83
1:A:96:LEU:CD1	1:D:430:LEU:HD12	2.09	0.82
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.61	0.82
1:A:95:TRP:CE3	1:A:97:ILE:HD11	2.15	0.82
1:B:95:TRP:CE3	1:B:97:ILE:HD11	2.14	0.82
1:C:549:TYR:O	1:C:590:THR:HG22	1.80	0.82
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.62	0.82
1:D:549:TYR:O	1:D:590:THR:HG22	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:THR:HG23	3:B:901:UDP:H5'2	1.62	0.81
1:C:320:ARG:HB2	1:C:320:ARG:NH1	1.94	0.81
1:C:95:TRP:CE3	1:C:97:ILE:HD11	2.15	0.81
1:D:482:ASN:HB3	1:D:484:ASN:HD21	1.46	0.81
1:B:59:ASP:HB2	1:B:96:LEU:HD21	1.63	0.80
1:C:482:ASN:HB3	1:C:484:ASN:HD21	1.46	0.80
1:D:550:GLY:HA3	1:D:590:THR:HG22	1.63	0.80
1:D:320:ARG:HB2	1:D:320:ARG:NH1	1.96	0.80
1:A:448:VAL:O	1:A:449:ASP:HB2	1.81	0.80
1:B:550:GLY:HA3	1:B:590:THR:HG22	1.64	0.80
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.63	0.80
1:C:448:VAL:O	1:C:449:ASP:HB2	1.83	0.79
1:A:539:ASP:O	1:A:540:LEU:HD23	1.83	0.78
1:B:448:VAL:O	1:B:449:ASP:HB2	1.80	0.78
1:A:484:ASN:H	1:A:484:ASN:HD22	1.32	0.78
1:D:448:VAL:O	1:D:449:ASP:HB2	1.82	0.78
1:B:17:VAL:HG21	1:B:47:GLY:HA3	1.67	0.77
1:C:482:ASN:HB3	1:C:484:ASN:ND2	1.99	0.77
1:D:95:TRP:CE3	1:D:97:ILE:HD11	2.18	0.77
1:A:482:ASN:HB3	1:A:484:ASN:HD21	1.48	0.77
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.14	0.77
1:D:532:GLY:O	1:D:535:SER:OG	2.03	0.77
1:B:532:GLY:O	1:B:535:SER:OG	2.03	0.76
1:A:552:TYR:HD1	1:A:571:TYR:CD2	2.04	0.76
1:D:482:ASN:HB3	1:D:484:ASN:ND2	2.01	0.76
1:B:482:ASN:HB3	1:B:484:ASN:HD21	1.47	0.76
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.16	0.76
1:B:399:ARG:HH22	1:D:308:ASP:HA	1.52	0.75
1:C:331:PHE:O	1:C:335:LEU:HD12	1.87	0.75
1:A:308:ASP:O	1:A:312:THR:HG23	1.87	0.74
1:A:429:ILE:HG12	1:C:397:ALA:HB1	1.68	0.74
1:A:17:VAL:HG21	1:A:47:GLY:HA3	1.69	0.74
1:B:482:ASN:HB3	1:B:484:ASN:ND2	2.02	0.74
1:C:552:TYR:HD1	1:C:571:TYR:CD2	2.06	0.74
1:B:484:ASN:ND2	1:B:484:ASN:H	1.86	0.73
1:A:484:ASN:ND2	1:A:484:ASN:H	1.83	0.73
1:B:308:ASP:O	1:B:312:THR:HG23	1.88	0.73
1:B:552:TYR:HD1	1:B:571:TYR:CD2	2.06	0.73
1:C:308:ASP:O	1:C:312:THR:HG23	1.89	0.73
1:D:552:TYR:HD1	1:D:571:TYR:CD2	2.07	0.73
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:HD22	1:B:133:ASN:H	1.36	0.72
1:C:133:ASN:HD22	1:C:133:ASN:H	1.35	0.72
1:A:532:GLY:O	1:A:535:SER:OG	2.06	0.72
1:D:447:MET:HG3	1:D:456:LEU:HD11	1.72	0.72
1:A:390:GLY:CA	1:C:386:THR:HG21	2.20	0.72
1:A:482:ASN:HB3	1:A:484:ASN:ND2	2.03	0.72
1:D:133:ASN:H	1:D:133:ASN:HD22	1.36	0.72
1:A:314:TYR:H	1:A:500:HIS:HD2	1.38	0.72
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.20	0.72
1:C:447:MET:HG3	1:C:456:LEU:HD11	1.72	0.72
1:D:484:ASN:H	1:D:484:ASN:ND2	1.88	0.71
1:B:399:ARG:NH2	1:D:308:ASP:HA	2.05	0.71
1:D:308:ASP:O	1:D:312:THR:HG23	1.90	0.71
1:C:484:ASN:ND2	1:C:484:ASN:H	1.88	0.71
1:B:484:ASN:H	1:B:484:ASN:HD22	1.36	0.71
1:C:314:TYR:H	1:C:500:HIS:HD2	1.39	0.71
1:D:484:ASN:HD22	1:D:484:ASN:H	1.38	0.71
1:A:386:THR:HG21	1:C:390:GLY:HA2	1.73	0.71
1:C:532:GLY:O	1:C:535:SER:OG	2.06	0.71
1:C:17:VAL:HG21	1:C:47:GLY:HA3	1.72	0.70
1:A:133:ASN:HD22	1:A:133:ASN:H	1.38	0.69
1:D:264:ASP:O	1:D:635:MET:HG3	1.91	0.69
1:A:447:MET:HG3	1:A:456:LEU:HD11	1.72	0.69
1:A:264:ASP:O	1:A:635:MET:HG3	1.92	0.69
1:D:17:VAL:HG21	1:D:47:GLY:HA3	1.75	0.69
1:A:386:THR:HG21	1:C:390:GLY:CA	2.23	0.69
1:C:95:TRP:CD2	1:C:97:ILE:HD11	2.28	0.68
1:B:447:MET:HG3	1:B:456:LEU:HD11	1.73	0.68
1:D:122:LEU:HD13	1:D:128:ILE:HB	1.75	0.68
1:B:264:ASP:O	1:B:635:MET:HG3	1.93	0.68
1:D:314:TYR:H	1:D:500:HIS:HD2	1.39	0.68
1:A:95:TRP:CD2	1:A:97:ILE:HD11	2.29	0.68
1:D:612:LEU:HD21	1:D:616:ARG:HH21	1.59	0.68
1:B:579:THR:HG23	1:B:582:GLN:OE1	1.95	0.68
1:C:122:LEU:HD13	1:C:128:ILE:HB	1.76	0.67
1:B:95:TRP:CD2	1:B:97:ILE:HD11	2.29	0.67
1:B:331:PHE:O	1:B:335:LEU:HD12	1.95	0.67
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.75	0.67
1:C:612:LEU:HD21	1:C:616:ARG:HH21	1.59	0.67
1:B:314:TYR:H	1:B:500:HIS:HD2	1.41	0.67
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:PHE:O	1:D:335:LEU:HD12	1.95	0.67
1:D:579:THR:HG23	1:D:582:GLN:OE1	1.95	0.67
1:C:579:THR:HG23	1:C:582:GLN:OE1	1.94	0.67
1:C:32:ALA:HB3	1:C:33:PRO:HD3	1.77	0.66
1:C:484:ASN:H	1:C:484:ASN:HD22	1.41	0.66
1:A:306:ASP:OD2	1:A:468:PRO:HB3	1.95	0.66
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.78	0.66
1:A:579:THR:HG23	1:A:582:GLN:OE1	1.95	0.66
1:A:331:PHE:O	1:A:335:LEU:HD12	1.95	0.66
1:C:480:PHE:HD1	3:C:901:UDP:C4	2.14	0.65
1:B:307:PHE:O	1:D:399:ARG:NH2	2.30	0.65
1:D:95:TRP:CD2	1:D:97:ILE:HD11	2.32	0.64
1:B:122:LEU:HD13	1:B:128:ILE:HB	1.77	0.64
1:B:612:LEU:HD21	1:B:616:ARG:HH21	1.61	0.64
1:C:264:ASP:O	1:C:635:MET:HG3	1.97	0.64
1:B:163:ILE:HB	1:B:186:VAL:HG12	1.79	0.64
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.79	0.64
1:A:163:ILE:HB	1:A:186:VAL:HG12	1.79	0.64
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.79	0.64
1:B:306:ASP:OD2	1:B:468:PRO:HB3	1.98	0.63
1:D:306:ASP:OD2	1:D:468:PRO:HB3	1.97	0.63
1:A:612:LEU:HD21	1:A:616:ARG:HH21	1.61	0.63
1:C:306:ASP:OD2	1:C:468:PRO:HB3	1.97	0.63
1:A:122:LEU:HD13	1:A:128:ILE:HB	1.81	0.62
1:D:213:LEU:C	1:D:213:LEU:HD12	2.20	0.62
1:B:17:VAL:CG2	1:B:47:GLY:HA3	2.28	0.62
1:A:623:ARG:HG3	1:A:628:GLU:O	2.00	0.62
1:C:6:GLN:NE2	1:C:625:LEU:HD21	2.16	0.61
1:A:17:VAL:CG2	1:A:47:GLY:HA3	2.30	0.61
1:D:567:GLN:HG2	1:D:571:TYR:CE1	2.36	0.61
1:A:208:ASP:OD1	1:A:209:PHE:N	2.33	0.61
1:A:193:HIS:O	1:A:194:ALA:HB2	2.01	0.61
1:C:344:VAL:C	1:C:346:GLY:H	2.04	0.60
1:D:6:GLN:NE2	1:D:625:LEU:HD21	2.16	0.60
1:B:455:ILE:O	1:B:459:ILE:HG23	2.02	0.60
1:A:442:ILE:HD12	1:A:459:ILE:HD11	1.83	0.60
1:B:6:GLN:NE2	1:B:625:LEU:HD21	2.17	0.60
1:D:455:ILE:O	1:D:459:ILE:HG23	2.01	0.60
1:C:567:GLN:HG2	1:C:571:TYR:CE1	2.37	0.60
1:B:623:ARG:HG3	1:B:628:GLU:O	2.00	0.60
1:C:442:ILE:HD12	1:C:459:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ILE:O	1:C:459:ILE:HG23	2.01	0.60
1:B:480:PHE:HD1	3:B:901:UDP:C4	2.20	0.60
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.67	0.60
1:B:567:GLN:HG2	1:B:571:TYR:CE1	2.36	0.60
1:B:208:ASP:OD1	1:B:209:PHE:N	2.33	0.60
1:D:344:VAL:C	1:D:346:GLY:H	2.04	0.60
1:A:213:LEU:C	1:A:213:LEU:HD12	2.21	0.60
1:C:213:LEU:C	1:C:213:LEU:HD12	2.23	0.60
1:A:344:VAL:C	1:A:346:GLY:H	2.04	0.59
1:A:6:GLN:NE2	1:A:625:LEU:HD21	2.17	0.59
1:B:213:LEU:C	1:B:213:LEU:HD12	2.23	0.59
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.66	0.59
1:A:305:PHE:HZ	1:A:309:LEU:HG	1.67	0.59
1:D:39:TYR:OH	1:D:610:ARG:NH1	2.35	0.59
1:B:487:ILE:HG22	1:B:488:LEU:N	2.17	0.59
1:D:442:ILE:HD12	1:D:459:ILE:HD11	1.84	0.59
1:D:487:ILE:HG22	1:D:488:LEU:N	2.18	0.59
1:A:487:ILE:HG22	1:A:488:LEU:N	2.18	0.59
1:B:442:ILE:HD12	1:B:459:ILE:HD11	1.83	0.59
1:A:96:LEU:HD11	1:D:430:LEU:HD12	1.85	0.58
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.85	0.58
1:B:344:VAL:C	1:B:346:GLY:H	2.05	0.58
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.39	0.58
1:B:80:LEU:HD22	1:B:90:PHE:CE1	2.39	0.58
1:A:567:GLN:HG2	1:A:571:TYR:CE1	2.38	0.58
1:A:455:ILE:O	1:A:459:ILE:HG23	2.03	0.58
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.36	0.58
1:B:425:LEU:O	1:B:429:ILE:HG13	2.04	0.58
1:C:17:VAL:CG2	1:C:47:GLY:HA3	2.33	0.58
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.35	0.58
1:A:74:ARG:NH1	1:A:77:GLN:OE1	2.36	0.58
1:C:479:GLU:OE2	1:C:479:GLU:HA	2.03	0.58
1:B:39:TYR:OH	1:B:610:ARG:NH1	2.37	0.58
1:B:479:GLU:HA	1:B:479:GLU:OE2	2.04	0.58
1:D:305:PHE:HZ	1:D:309:LEU:HG	1.66	0.57
1:B:12:GLU:OE2	1:B:168:HIS:HE1	1.86	0.57
1:D:208:ASP:OD1	1:D:209:PHE:N	2.37	0.57
1:A:181:LYS:C	1:A:181:LYS:HD3	2.25	0.57
1:A:12:GLU:OE2	1:A:168:HIS:HE1	1.86	0.57
1:C:208:ASP:OD1	1:C:209:PHE:N	2.36	0.57
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:ASN:HB2	1:C:637:ALA:H	1.70	0.57
1:D:3:ARG:NH1	1:D:185:ASP:OD2	2.37	0.57
1:B:537:MET:HG3	1:B:551:ILE:HD13	1.87	0.57
1:D:20:ARG:NH1	2:D:801:SO4:O3	2.38	0.57
1:A:458:LYS:HE3	1:A:461:GLN:OE1	2.04	0.57
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.87	0.56
1:D:623:ARG:HG3	1:D:628:GLU:O	2.05	0.56
1:A:146:THR:O	1:A:149:TRP:HB3	2.05	0.56
1:C:133:ASN:H	1:C:133:ASN:ND2	2.03	0.56
1:A:537:MET:HG3	1:A:551:ILE:HD13	1.86	0.56
1:A:449:ASP:OD2	1:A:452:ASN:HB2	2.05	0.56
1:D:74:ARG:NH1	1:D:77:GLN:OE1	2.39	0.56
1:D:458:LYS:HE3	1:D:461:GLN:OE1	2.06	0.56
1:B:181:LYS:HD3	1:B:181:LYS:C	2.26	0.56
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.05	0.56
1:B:272:ASN:O	1:B:275:LYS:HB3	2.05	0.56
1:D:12:GLU:OE2	1:D:168:HIS:HE1	1.89	0.56
1:D:189:ILE:HD11	1:D:610:ARG:HA	1.88	0.56
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.88	0.56
1:C:487:ILE:HG22	1:C:488:LEU:N	2.19	0.56
1:A:479:GLU:HA	1:A:479:GLU:OE2	2.05	0.56
1:A:314:TYR:H	1:A:500:HIS:CD2	2.23	0.56
1:B:74:ARG:NH1	1:B:77:GLN:OE1	2.38	0.56
1:B:449:ASP:OD2	1:B:452:ASN:HB2	2.05	0.56
1:A:39:TYR:OH	1:A:610:ARG:NH1	2.39	0.56
1:D:323:TYR:OH	1:D:458:LYS:HG3	2.05	0.56
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.34	0.56
1:D:80:LEU:HD22	1:D:90:PHE:CE1	2.41	0.56
1:C:179:CYS:HA	1:C:184:ILE:HG13	1.88	0.56
1:C:181:LYS:C	1:C:181:LYS:HD3	2.26	0.56
1:B:323:TYR:OH	1:B:458:LYS:HG3	2.06	0.56
1:A:634:ASN:HB2	1:A:637:ALA:H	1.70	0.56
1:C:572:MET:O	1:C:576:VAL:HG23	2.07	0.55
1:C:74:ARG:NH1	1:C:77:GLN:OE1	2.39	0.55
1:C:514:THR:HG23	3:C:901:UDP:H3'	1.88	0.55
1:B:634:ASN:HB2	1:B:637:ALA:H	1.70	0.55
1:A:323:TYR:OH	1:A:458:LYS:HG3	2.05	0.55
1:D:634:ASN:HB2	1:D:637:ALA:H	1.70	0.55
1:C:314:TYR:H	1:C:500:HIS:CD2	2.23	0.55
1:D:612:LEU:HD21	1:D:616:ARG:NH2	2.21	0.55
1:C:80:LEU:HD22	1:C:90:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ILE:HG23	1:C:416:LEU:HD13	1.89	0.55
1:A:394:PHE:HE1	1:C:379:GLU:HG3	1.71	0.55
1:C:612:LEU:HD21	1:C:616:ARG:NH2	2.21	0.55
1:B:179:CYS:HA	1:B:184:ILE:HG13	1.88	0.55
1:C:537:MET:HG3	1:C:551:ILE:HD13	1.88	0.55
1:A:399:ARG:NH2	1:C:307:PHE:O	2.40	0.55
1:B:330:MET:HE3	1:B:568:LEU:HD12	1.88	0.54
1:A:389:ILE:HG23	1:A:416:LEU:HD13	1.88	0.54
1:B:389:ILE:HG23	1:B:416:LEU:HD13	1.87	0.54
1:D:272:ASN:O	1:D:275:LYS:HB3	2.07	0.54
1:C:320:ARG:NH1	1:C:320:ARG:CB	2.59	0.54
1:B:458:LYS:HE3	1:B:461:GLN:OE1	2.06	0.54
1:C:12:GLU:OE2	1:C:168:HIS:HE1	1.90	0.54
1:B:612:LEU:HD21	1:B:616:ARG:NH2	2.23	0.54
1:D:193:HIS:O	1:D:194:ALA:HB2	2.08	0.54
1:A:612:LEU:HD21	1:A:616:ARG:NH2	2.23	0.54
1:D:389:ILE:HG23	1:D:416:LEU:HD13	1.90	0.54
1:C:458:LYS:HE3	1:C:461:GLN:OE1	2.07	0.54
1:D:479:GLU:HA	1:D:479:GLU:OE2	2.07	0.54
1:D:537:MET:HG3	1:D:551:ILE:HD13	1.88	0.54
1:D:133:ASN:ND2	1:D:133:ASN:H	2.04	0.54
1:D:17:VAL:CG2	1:D:47:GLY:HA3	2.37	0.54
1:A:127:GLY:O	1:A:129:PRO:HD3	2.07	0.54
1:C:127:GLY:O	1:C:129:PRO:HD3	2.08	0.54
1:A:272:ASN:O	1:A:275:LYS:HB3	2.08	0.53
1:D:425:LEU:O	1:D:429:ILE:HG13	2.09	0.53
1:C:449:ASP:OD2	1:C:452:ASN:HB2	2.08	0.53
1:A:16:GLU:O	1:A:17:VAL:C	2.46	0.53
1:C:330:MET:HE3	1:C:568:LEU:HD12	1.90	0.53
1:B:193:HIS:O	1:B:194:ALA:HB2	2.06	0.53
1:A:12:GLU:HG3	1:A:166:HIS:HB3	1.91	0.53
1:D:449:ASP:OD2	1:D:452:ASN:HB2	2.08	0.53
1:C:16:GLU:O	1:C:17:VAL:C	2.46	0.53
1:C:623:ARG:HG3	1:C:628:GLU:O	2.08	0.53
1:A:425:LEU:O	1:A:429:ILE:HG13	2.09	0.53
1:C:312:THR:HG22	1:C:350:THR:HB	1.90	0.53
1:C:272:ASN:O	1:C:275:LYS:HB3	2.08	0.53
1:B:127:GLY:O	1:B:129:PRO:HD3	2.08	0.53
1:C:12:GLU:HG3	1:C:166:HIS:HB3	1.91	0.53
1:B:465:PHE:O	1:B:466:ASN:HB2	2.09	0.53
1:D:181:LYS:HD3	1:D:181:LYS:C	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ARG:HH11	1:D:86:ARG:HB3	1.74	0.53
1:D:113:GLY:C	1:D:115:SER:H	2.13	0.52
1:C:425:LEU:O	1:C:429:ILE:HG13	2.10	0.52
1:A:480:PHE:HD1	3:A:901:UDP:C4	2.27	0.52
1:D:312:THR:HG22	1:D:350:THR:HB	1.91	0.52
1:A:386:THR:CG2	1:C:390:GLY:HA2	2.39	0.52
1:D:179:CYS:HA	1:D:184:ILE:HG13	1.92	0.52
1:D:12:GLU:HG3	1:D:166:HIS:HB3	1.92	0.52
1:A:179:CYS:HA	1:A:184:ILE:HG13	1.91	0.52
1:B:16:GLU:O	1:B:17:VAL:C	2.46	0.52
1:B:49:LEU:HD11	1:B:54:TYR:CG	2.45	0.52
1:D:330:MET:HE3	1:D:568:LEU:HD12	1.90	0.51
1:D:49:LEU:HD11	1:D:54:TYR:CG	2.44	0.51
1:D:320:ARG:CB	1:D:320:ARG:NH1	2.60	0.51
1:A:109:ASP:OD1	1:A:112:ARG:NH1	2.43	0.51
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.46	0.51
1:B:146:THR:O	1:B:149:TRP:HB3	2.09	0.51
1:A:113:GLY:C	1:A:115:SER:H	2.13	0.51
1:A:150:PHE:O	1:A:154:VAL:HG23	2.11	0.51
1:C:86:ARG:HH11	1:C:86:ARG:HB3	1.75	0.51
1:A:320:ARG:NH1	1:A:320:ARG:CB	2.56	0.51
1:B:133:ASN:ND2	1:B:133:ASN:H	2.05	0.51
1:C:465:PHE:O	1:C:466:ASN:HB2	2.10	0.51
1:D:109:ASP:OD1	1:D:112:ARG:NH1	2.44	0.51
1:B:484:ASN:HD22	1:B:484:ASN:N	2.08	0.51
1:B:109:ASP:OD1	1:B:112:ARG:NH1	2.43	0.51
1:C:49:LEU:HD11	1:C:54:TYR:CG	2.45	0.51
1:D:572:MET:O	1:D:576:VAL:HG23	2.11	0.51
1:C:357:MET:O	1:C:478:PRO:HA	2.11	0.51
1:C:109:ASP:OD1	1:C:112:ARG:NH1	2.43	0.51
1:A:330:MET:HE3	1:A:568:LEU:HD12	1.91	0.51
1:D:16:GLU:O	1:D:17:VAL:C	2.49	0.51
1:C:39:TYR:OH	1:C:610:ARG:NH1	2.44	0.51
1:A:572:MET:O	1:A:576:VAL:HG23	2.11	0.51
1:C:320:ARG:NH1	3:C:901:UDP:O1A	2.45	0.51
1:A:49:LEU:HD11	1:A:54:TYR:CG	2.46	0.51
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.46	0.50
1:D:351:VAL:HB	1:D:472:VAL:HG12	1.93	0.50
1:B:320:ARG:CB	1:B:320:ARG:NH1	2.57	0.50
1:C:448:VAL:O	1:C:449:ASP:CB	2.57	0.50
1:A:86:ARG:HH11	1:A:86:ARG:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:C	1:B:115:SER:H	2.13	0.50
1:C:123:TRP:O	1:C:127:GLY:HA2	2.12	0.50
1:C:552:TYR:CD2	1:C:552:TYR:N	2.79	0.50
1:B:314:TYR:H	1:B:500:HIS:CD2	2.25	0.50
1:A:394:PHE:CE1	1:C:379:GLU:HG3	2.46	0.50
1:C:586:GLN:O	1:C:589:ARG:N	2.44	0.50
1:D:127:GLY:O	1:D:129:PRO:HD3	2.11	0.50
1:D:523:VAL:HG12	1:D:524:PRO:O	2.11	0.50
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.77	0.49
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.47	0.49
1:D:634:ASN:H	1:D:637:ALA:HB3	1.78	0.49
1:D:586:GLN:O	1:D:589:ARG:N	2.45	0.49
1:A:312:THR:HG22	1:A:350:THR:HB	1.94	0.49
1:A:133:ASN:ND2	1:A:133:ASN:H	2.06	0.49
1:D:267:LEU:HB3	1:D:606:TYR:CE2	2.47	0.49
1:C:193:HIS:O	1:C:194:ALA:HB2	2.11	0.49
1:A:565:VAL:O	1:A:569:VAL:HG23	2.12	0.49
1:C:227:ILE:CG2	1:C:227:ILE:O	2.61	0.49
1:B:358:PRO:HG3	1:B:480:PHE:CZ	2.47	0.49
1:B:448:VAL:O	1:B:449:ASP:CB	2.55	0.49
1:B:12:GLU:HB3	1:B:45:LEU:HD23	1.94	0.49
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.47	0.49
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.94	0.49
1:A:330:MET:CE	1:A:568:LEU:HD12	2.43	0.49
1:C:351:VAL:HB	1:C:472:VAL:HG12	1.95	0.49
1:B:330:MET:CE	1:B:568:LEU:HD12	2.42	0.49
1:B:539:ASP:O	1:B:540:LEU:HD23	2.13	0.49
1:B:585:ASN:HB3	1:B:589:ARG:NH2	2.28	0.49
1:A:465:PHE:O	1:A:466:ASN:HB2	2.13	0.49
1:B:312:THR:HG22	1:B:350:THR:HB	1.94	0.49
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.95	0.49
1:C:330:MET:CE	1:C:568:LEU:HD12	2.42	0.49
1:D:227:ILE:O	1:D:227:ILE:CG2	2.61	0.49
1:B:398:ILE:HG12	1:D:298:ARG:HD3	1.94	0.49
1:A:351:VAL:HB	1:A:472:VAL:HG12	1.94	0.48
1:C:565:VAL:O	1:C:569:VAL:HG23	2.13	0.48
1:B:361:ASN:HA	1:B:448:VAL:HG23	1.95	0.48
1:C:113:GLY:C	1:C:115:SER:H	2.16	0.48
1:A:358:PRO:HG3	1:A:480:PHE:CZ	2.48	0.48
1:B:351:VAL:HB	1:B:472:VAL:HG12	1.94	0.48
1:D:528:THR:O	1:D:534:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:GLN:HG2	1:D:571:TYR:HE1	1.78	0.48
1:D:330:MET:CE	1:D:568:LEU:HD12	2.43	0.48
1:D:357:MET:O	1:D:478:PRO:HA	2.14	0.48
1:B:128:ILE:HG21	1:B:233:ILE:HG12	1.94	0.48
1:B:123:TRP:O	1:B:127:GLY:HA2	2.13	0.48
1:C:267:LEU:HB3	1:C:606:TYR:CE2	2.49	0.48
1:A:514:THR:HG23	3:A:901:UDP:H5'2	1.96	0.48
1:C:585:ASN:HB3	1:C:589:ARG:NH2	2.28	0.48
1:B:267:LEU:HB3	1:B:606:TYR:CE2	2.48	0.48
1:D:146:THR:O	1:D:149:TRP:HB3	2.14	0.48
1:A:96:LEU:HD11	1:D:430:LEU:CD1	2.44	0.48
1:C:484:ASN:HD22	1:C:484:ASN:N	2.11	0.48
1:D:314:TYR:H	1:D:500:HIS:CD2	2.24	0.48
1:D:585:ASN:HB3	1:D:589:ARG:NH2	2.29	0.48
1:B:20:ARG:NH1	2:B:801:SO4:O4	2.46	0.48
1:A:100:ALA:HB2	1:D:423:VAL:HG21	1.94	0.48
1:D:539:ASP:O	1:D:540:LEU:HD23	2.14	0.48
1:C:34:ILE:HD12	1:C:34:ILE:HA	1.74	0.48
1:C:358:PRO:HG3	1:C:480:PHE:CZ	2.48	0.48
1:A:448:VAL:O	1:A:449:ASP:CB	2.55	0.48
1:D:361:ASN:HA	1:D:448:VAL:HG23	1.95	0.48
1:D:12:GLU:HB3	1:D:45:LEU:HD23	1.96	0.48
1:B:192:THR:HG22	1:B:246:THR:HG22	1.96	0.48
1:B:31:LYS:O	1:B:35:THR:HG23	2.14	0.48
1:D:34:ILE:HD12	1:D:34:ILE:HA	1.77	0.48
1:B:34:ILE:HA	1:B:34:ILE:HD12	1.76	0.48
1:D:174:VAL:O	1:D:177:PRO:HD2	2.14	0.48
1:D:358:PRO:HG3	1:D:480:PHE:CZ	2.48	0.48
1:A:267:LEU:HB3	1:A:606:TYR:CE2	2.49	0.48
1:B:357:MET:O	1:B:478:PRO:HA	2.13	0.48
1:A:361:ASN:HA	1:A:448:VAL:HG23	1.96	0.47
1:D:128:ILE:HG21	1:D:233:ILE:HG12	1.96	0.47
1:D:552:TYR:N	1:D:552:TYR:CD2	2.82	0.47
1:C:550:GLY:HA3	1:C:590:THR:HG21	1.96	0.47
1:D:183:ARG:HB2	1:D:183:ARG:HE	1.47	0.47
1:B:74:ARG:HA	1:B:74:ARG:HD3	1.64	0.47
1:C:490:LEU:HD22	1:C:494:GLU:HB3	1.97	0.47
1:B:490:LEU:HD22	1:B:494:GLU:HB3	1.96	0.47
1:C:344:VAL:C	1:C:346:GLY:N	2.68	0.47
1:A:66:PRO:O	1:A:74:ARG:NH2	2.47	0.47
1:D:74:ARG:N	1:D:75:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:ALA:HB1	1:C:561:PRO:HD2	1.97	0.47
1:C:361:ASN:HA	1:C:448:VAL:HG23	1.97	0.47
1:B:539:ASP:C	1:B:540:LEU:HG	2.34	0.47
1:D:565:VAL:O	1:D:569:VAL:HG23	2.15	0.47
1:B:344:VAL:C	1:B:346:GLY:N	2.69	0.47
1:B:586:GLN:O	1:B:589:ARG:N	2.47	0.47
1:B:634:ASN:H	1:B:637:ALA:HB3	1.80	0.47
1:A:585:ASN:HB3	1:A:589:ARG:NH2	2.29	0.47
1:B:150:PHE:O	1:B:154:VAL:HG23	2.14	0.47
1:D:465:PHE:O	1:D:466:ASN:HB2	2.15	0.47
1:A:523:VAL:HG12	1:A:524:PRO:O	2.15	0.46
1:B:572:MET:O	1:B:576:VAL:HG23	2.15	0.46
1:B:560:ALA:HB1	1:B:561:PRO:HD2	1.97	0.46
1:D:344:VAL:C	1:D:346:GLY:N	2.69	0.46
1:D:321:TYR:CD1	1:D:321:TYR:C	2.88	0.46
1:D:484:ASN:N	1:D:484:ASN:HD22	2.11	0.46
1:C:174:VAL:O	1:C:177:PRO:HD2	2.15	0.46
1:A:344:VAL:C	1:A:346:GLY:N	2.68	0.46
1:A:537:MET:CG	1:A:551:ILE:HD13	2.46	0.46
1:D:73:MET:C	1:D:75:PRO:HD2	2.36	0.46
1:C:227:ILE:HG22	1:C:227:ILE:O	2.15	0.46
1:A:586:GLN:O	1:A:589:ARG:N	2.46	0.46
1:A:439:LEU:HD22	1:A:467:SER:HA	1.98	0.46
1:A:552:TYR:N	1:A:552:TYR:CD2	2.83	0.46
1:C:567:GLN:HG2	1:C:571:TYR:HE1	1.79	0.46
1:D:321:TYR:HD1	1:D:321:TYR:C	2.18	0.46
1:D:123:TRP:O	1:D:127:GLY:HA2	2.15	0.46
1:A:235:ARG:HH21	1:A:260:LYS:HG3	1.80	0.46
1:C:321:TYR:C	1:C:321:TYR:HD1	2.19	0.46
1:B:537:MET:CG	1:B:551:ILE:HD13	2.46	0.46
1:C:321:TYR:CD1	1:C:321:TYR:C	2.89	0.46
1:B:528:THR:O	1:B:534:GLY:HA3	2.16	0.46
1:D:560:ALA:HB1	1:D:561:PRO:HD2	1.98	0.46
1:D:490:LEU:HD22	1:D:494:GLU:HB3	1.98	0.46
1:B:523:VAL:HG12	1:B:524:PRO:O	2.16	0.46
1:D:289:LYS:HD2	1:D:289:LYS:N	2.30	0.46
1:C:192:THR:HG22	1:C:246:THR:HG22	1.98	0.45
1:C:289:LYS:HD2	1:C:289:LYS:N	2.30	0.45
1:B:227:ILE:HD13	1:B:227:ILE:HA	1.74	0.45
1:A:192:THR:HG22	1:A:246:THR:HG22	1.98	0.45
1:A:34:ILE:HD12	1:A:34:ILE:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:VAL:HG23	1:D:464:LEU:HG	1.98	0.45
1:A:320:ARG:HB3	1:A:320:ARG:HH11	1.74	0.45
1:B:552:TYR:N	1:B:552:TYR:CD2	2.84	0.45
1:C:302:HIS:O	1:C:434:ARG:HD2	2.16	0.45
1:A:289:LYS:N	1:A:289:LYS:HD2	2.32	0.45
1:C:235:ARG:HH21	1:C:260:LYS:HG3	1.81	0.45
1:D:192:THR:HG22	1:D:246:THR:HG22	1.98	0.45
1:A:484:ASN:HD22	1:A:484:ASN:N	2.06	0.45
1:A:74:ARG:HB2	1:A:75:PRO:HD3	1.99	0.45
1:A:266:ILE:HA	1:A:266:ILE:HD13	1.74	0.45
1:A:490:LEU:HD22	1:A:494:GLU:HB3	1.98	0.45
1:B:227:ILE:O	1:B:227:ILE:CG2	2.63	0.45
1:B:235:ARG:HH21	1:B:260:LYS:HG3	1.81	0.45
1:C:523:VAL:HG12	1:C:524:PRO:O	2.16	0.45
1:C:66:PRO:O	1:C:74:ARG:NH2	2.48	0.45
1:A:302:HIS:O	1:A:434:ARG:HD2	2.16	0.45
1:A:567:GLN:HG2	1:A:571:TYR:HE1	1.80	0.45
1:C:634:ASN:H	1:C:637:ALA:HB3	1.81	0.45
1:B:74:ARG:HB2	1:B:75:PRO:HD3	1.99	0.45
1:C:74:ARG:HD3	1:C:74:ARG:HA	1.61	0.45
1:A:31:LYS:O	1:A:35:THR:HG23	2.17	0.45
1:C:528:THR:O	1:C:534:GLY:HA3	2.16	0.45
1:D:31:LYS:O	1:D:35:THR:HG23	2.16	0.45
1:D:320:ARG:HB3	1:D:320:ARG:HH11	1.75	0.45
1:C:484:ASN:ND2	1:C:484:ASN:N	2.61	0.45
1:D:552:TYR:HD1	1:D:571:TYR:HD2	1.62	0.45
1:B:66:PRO:O	1:B:74:ARG:NH2	2.48	0.45
1:D:31:LYS:HZ3	1:D:35:THR:HG21	1.82	0.45
1:B:29:LYS:HG3	1:B:97:ILE:CG2	2.30	0.44
1:A:634:ASN:H	1:A:637:ALA:HB3	1.82	0.44
1:C:146:THR:O	1:C:149:TRP:HB3	2.17	0.44
1:C:552:TYR:HD1	1:C:571:TYR:HD2	1.62	0.44
1:C:74:ARG:N	1:C:75:PRO:CD	2.80	0.44
1:D:331:PHE:CE1	1:D:503:VAL:HB	2.52	0.44
1:A:193:HIS:O	1:A:194:ALA:CB	2.66	0.44
1:D:227:ILE:O	1:D:227:ILE:HG22	2.15	0.44
1:A:462:VAL:HG23	1:A:464:LEU:HG	1.99	0.44
1:C:480:PHE:HD1	3:C:901:UDP:C5	2.35	0.44
1:A:593:LEU:HA	1:A:593:LEU:HD23	1.84	0.44
1:B:423:VAL:HG12	1:B:424:MET:N	2.32	0.44
1:B:400:TYR:HA	1:B:401:PRO:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:PRO:O	1:A:518:CYS:HB3	2.18	0.44
1:B:95:TRP:CZ3	1:B:97:ILE:HD11	2.51	0.44
1:D:480:PHE:HD1	3:D:901:UDP:C4	2.36	0.44
1:D:320:ARG:NH1	3:D:901:UDP:O2A	2.50	0.44
1:D:550:GLY:HA3	1:D:590:THR:HG21	1.99	0.44
1:C:331:PHE:CE1	1:C:503:VAL:HB	2.52	0.44
1:D:515:PRO:O	1:D:518:CYS:HB3	2.17	0.44
1:D:439:LEU:HD22	1:D:467:SER:HA	1.98	0.44
1:B:289:LYS:N	1:B:289:LYS:HD2	2.32	0.44
1:B:567:GLN:HG2	1:B:571:TYR:HE1	1.79	0.44
1:C:31:LYS:HZ3	1:C:35:THR:HG21	1.83	0.44
1:D:623:ARG:HE	1:D:623:ARG:HB2	1.66	0.44
1:D:537:MET:CG	1:D:551:ILE:HD13	2.47	0.44
1:D:235:ARG:HH21	1:D:260:LYS:HG3	1.82	0.44
1:B:565:VAL:O	1:B:569:VAL:HG23	2.18	0.44
1:C:537:MET:CG	1:C:551:ILE:HD13	2.48	0.44
1:D:150:PHE:O	1:D:154:VAL:HG23	2.17	0.44
1:B:462:VAL:HG23	1:B:464:LEU:HG	2.00	0.44
1:D:302:HIS:O	1:D:434:ARG:HD2	2.17	0.44
1:A:209:PHE:O	1:A:211:ASN:N	2.52	0.43
1:B:515:PRO:O	1:B:518:CYS:HB3	2.18	0.43
1:C:307:PHE:HD1	1:C:312:THR:HG21	1.83	0.43
1:A:174:VAL:O	1:A:177:PRO:HD2	2.18	0.43
1:C:150:PHE:O	1:C:154:VAL:HG23	2.19	0.43
1:A:95:TRP:CZ3	1:A:97:ILE:HD11	2.52	0.43
1:C:128:ILE:HG21	1:C:233:ILE:HG12	1.99	0.43
1:B:74:ARG:N	1:B:75:PRO:CD	2.81	0.43
1:A:123:TRP:O	1:A:127:GLY:HA2	2.18	0.43
1:D:307:PHE:HD1	1:D:312:THR:HG21	1.83	0.43
1:A:487:ILE:HG22	1:A:488:LEU:HB2	2.00	0.43
1:D:74:ARG:HB2	1:D:75:PRO:HD3	2.00	0.43
1:C:515:PRO:O	1:C:518:CYS:HB3	2.19	0.43
1:A:590:THR:O	1:A:593:LEU:HB2	2.19	0.43
1:A:183:ARG:HE	1:A:183:ARG:HB2	1.47	0.43
1:C:73:MET:C	1:C:75:PRO:HD2	2.39	0.43
1:C:266:ILE:HG22	1:C:268:PRO:HD3	2.01	0.43
1:C:462:VAL:HG23	1:C:464:LEU:HG	2.00	0.43
1:D:514:THR:HG23	3:D:901:UDP:H3'	2.01	0.43
1:C:264:ASP:CG	1:C:616:ARG:HH22	2.22	0.43
1:A:560:ALA:HB1	1:A:561:PRO:HD2	1.99	0.43
1:A:227:ILE:CG2	1:A:227:ILE:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:N	1:A:75:PRO:CD	2.81	0.43
1:A:472:VAL:HG23	1:A:472:VAL:O	2.19	0.43
1:A:440:PRO:HA	1:A:441:PRO:HD3	1.93	0.43
1:B:343:LYS:HD3	1:B:469:SER:O	2.19	0.43
1:D:266:ILE:HG22	1:D:268:PRO:HD3	2.01	0.43
1:B:31:LYS:HZ3	1:B:35:THR:HG21	1.83	0.43
1:A:169:GLU:HG3	1:A:170:TRP:H	1.84	0.43
1:B:302:HIS:O	1:B:434:ARG:HD2	2.18	0.43
1:B:40:LYS:HB3	1:B:41:ASP:H	1.62	0.43
1:A:552:TYR:HD1	1:A:571:TYR:HD2	1.59	0.43
1:B:331:PHE:CE1	1:B:503:VAL:HB	2.53	0.43
1:A:266:ILE:HG22	1:A:268:PRO:HD3	1.99	0.43
1:B:439:LEU:HD22	1:B:467:SER:HA	2.00	0.43
1:C:490:LEU:HD13	1:C:495:PHE:HA	2.01	0.42
1:A:398:ILE:HA	1:A:398:ILE:HD12	1.91	0.42
1:B:264:ASP:CG	1:B:616:ARG:HH22	2.22	0.42
1:D:533:PHE:O	1:D:537:MET:HB2	2.19	0.42
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.73	0.42
1:D:264:ASP:CG	1:D:616:ARG:HH22	2.22	0.42
1:B:487:ILE:HG22	1:B:488:LEU:HB2	2.02	0.42
1:A:51:LYS:HE3	1:A:107:ASP:OD1	2.19	0.42
1:C:503:VAL:O	1:C:505:PRO:HD3	2.18	0.42
1:B:430:LEU:HA	1:B:430:LEU:HD23	1.92	0.42
1:A:73:MET:C	1:A:75:PRO:HD2	2.40	0.42
1:A:184:ILE:H	1:A:184:ILE:HG12	1.65	0.42
1:C:439:LEU:HD22	1:C:467:SER:HA	2.00	0.42
1:C:5:LEU:HD23	1:C:5:LEU:N	2.34	0.42
1:B:499:CYS:O	1:B:587:ARG:NH2	2.53	0.42
1:B:623:ARG:HB2	1:B:623:ARG:HE	1.66	0.42
1:D:209:PHE:O	1:D:211:ASN:N	2.53	0.42
1:D:74:ARG:HA	1:D:74:ARG:HD3	1.64	0.42
1:B:266:ILE:HG22	1:B:268:PRO:HD3	2.01	0.42
1:A:40:LYS:HB3	1:A:41:ASP:H	1.60	0.42
1:C:29:LYS:HG3	1:C:97:ILE:CG2	2.29	0.42
1:B:590:THR:O	1:B:593:LEU:HB2	2.20	0.42
1:B:608:LYS:HB2	1:B:635:MET:HE3	2.01	0.42
1:C:487:ILE:HG22	1:C:488:LEU:HB2	2.01	0.42
1:C:74:ARG:HB2	1:C:75:PRO:HD3	2.01	0.42
1:C:31:LYS:O	1:C:35:THR:HG23	2.20	0.42
1:D:210:TYR:CE1	1:D:250:ILE:HD11	2.54	0.42
1:A:331:PHE:CE1	1:A:503:VAL:HB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:TRP:CZ3	1:C:97:ILE:HD11	2.53	0.42
1:D:608:LYS:HB2	1:D:635:MET:HE3	2.02	0.42
1:B:227:ILE:O	1:B:227:ILE:HG22	2.18	0.42
1:D:111:VAL:HG13	1:D:111:VAL:O	2.20	0.42
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.84	0.41
1:D:266:ILE:HG22	1:D:268:PRO:HG3	2.02	0.41
1:B:471:ARG:NE	1:B:471:ARG:HA	2.34	0.41
1:A:229:HIS:O	1:A:233:ILE:HG13	2.19	0.41
1:C:29:LYS:HE3	1:C:97:ILE:CG2	2.50	0.41
1:D:39:TYR:OH	1:D:610:ARG:HD2	2.20	0.41
1:A:490:LEU:HD13	1:A:495:PHE:HA	2.02	0.41
1:B:51:LYS:HE3	1:B:107:ASP:OD1	2.20	0.41
1:B:29:LYS:HE3	1:B:97:ILE:CG2	2.51	0.41
1:A:29:LYS:HG3	1:A:97:ILE:CG2	2.32	0.41
1:C:209:PHE:O	1:C:211:ASN:N	2.53	0.41
1:B:73:MET:C	1:B:75:PRO:HD2	2.40	0.41
1:A:343:LYS:HD3	1:A:469:SER:O	2.19	0.41
1:B:169:GLU:HG3	1:B:170:TRP:H	1.85	0.41
1:D:366:VAL:HG12	1:D:367:GLU:N	2.34	0.41
1:C:430:LEU:HD23	1:C:430:LEU:HA	1.88	0.41
1:B:285:LEU:HA	1:B:285:LEU:HD23	1.91	0.41
1:D:448:VAL:O	1:D:449:ASP:CB	2.57	0.41
1:A:264:ASP:CG	1:A:616:ARG:HH22	2.23	0.41
1:D:309:LEU:HA	1:D:309:LEU:HD23	1.83	0.41
1:D:423:VAL:HG12	1:D:424:MET:N	2.35	0.41
1:A:357:MET:O	1:A:478:PRO:HA	2.19	0.41
1:A:29:LYS:HE3	1:A:97:ILE:CG2	2.50	0.41
1:B:319:GLY:O	1:B:358:PRO:HD3	2.20	0.41
1:B:503:VAL:O	1:B:505:PRO:HD3	2.21	0.41
1:A:39:TYR:OH	1:A:610:ARG:HD2	2.20	0.41
1:B:209:PHE:O	1:B:211:ASN:N	2.53	0.41
1:A:344:VAL:O	1:A:346:GLY:N	2.54	0.41
1:B:109:ASP:C	1:B:111:VAL:H	2.24	0.41
1:C:210:TYR:CE1	1:C:250:ILE:HD11	2.55	0.41
1:C:593:LEU:HD23	1:C:593:LEU:HA	1.87	0.41
1:A:307:PHE:HD1	1:A:312:THR:HG21	1.84	0.41
1:D:487:ILE:HG22	1:D:488:LEU:HB2	2.03	0.41
1:B:39:TYR:OH	1:B:610:ARG:HD2	2.20	0.41
1:D:227:ILE:HA	1:D:227:ILE:HD13	1.72	0.41
1:C:326:LYS:HA	1:C:326:LYS:HD3	1.89	0.41
1:D:40:LYS:HB3	1:D:41:ASP:H	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:CYS:O	1:C:587:ARG:NH2	2.53	0.41
1:D:66:PRO:O	1:D:74:ARG:NH2	2.47	0.41
1:B:490:LEU:HD13	1:B:495:PHE:HA	2.03	0.41
1:B:266:ILE:HD13	1:B:266:ILE:HA	1.78	0.41
1:B:174:VAL:O	1:B:177:PRO:HD2	2.20	0.41
1:D:307:PHE:CD1	1:D:312:THR:HG21	2.56	0.41
1:D:430:LEU:HA	1:D:430:LEU:HD23	1.86	0.41
1:D:535:SER:HG	1:D:536:TYR:H	1.69	0.41
1:A:331:PHE:O	1:A:335:LEU:CD1	2.68	0.41
1:A:266:ILE:HG22	1:A:268:PRO:HG3	2.03	0.41
1:A:528:THR:O	1:A:534:GLY:HA3	2.21	0.41
1:C:299:GLY:HA2	1:C:375:VAL:HG21	2.02	0.41
1:B:183:ARG:HB2	1:B:183:ARG:HE	1.47	0.41
1:B:5:LEU:N	1:B:5:LEU:HD23	2.35	0.41
1:B:593:LEU:HD23	1:B:593:LEU:HA	1.86	0.40
1:C:307:PHE:CD1	1:C:312:THR:HG21	2.56	0.40
1:A:471:ARG:HA	1:A:471:ARG:NE	2.36	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.88	0.40
1:C:134:ASP:OD2	1:C:137:THR:HG23	2.21	0.40
1:A:103:VAL:CG1	1:A:105:LEU:HG	2.51	0.40
1:A:5:LEU:HD23	1:A:5:LEU:N	2.36	0.40
1:C:632:ASP:OD2	1:C:632:ASP:C	2.60	0.40
1:A:539:ASP:C	1:A:540:LEU:HG	2.42	0.40
1:B:266:ILE:HG22	1:B:268:PRO:HG3	2.02	0.40
1:C:286:HIS:ND1	1:C:587:ARG:NH2	2.70	0.40
1:B:250:ILE:HG22	1:B:532:GLY:HA2	2.02	0.40
1:B:307:PHE:CD1	1:B:312:THR:HG21	2.57	0.40
1:B:126:VAL:HB	1:B:128:ILE:HG13	2.04	0.40
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.93	0.40
1:B:632:ASP:OD2	1:B:632:ASP:C	2.60	0.40
1:D:484:ASN:N	1:D:484:ASN:ND2	2.61	0.40
1:B:210:TYR:CE1	1:B:250:ILE:HD11	2.56	0.40
1:B:552:TYR:HD1	1:B:571:TYR:HD2	1.61	0.40
1:A:113:GLY:O	1:A:115:SER:N	2.54	0.40
1:D:490:LEU:HD13	1:D:495:PHE:HA	2.04	0.40
1:B:103:VAL:CG1	1:B:105:LEU:HG	2.52	0.40
1:A:261:ARG:O	1:A:263:PRO:HD3	2.22	0.40
1:A:423:VAL:HG12	1:A:424:MET:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	601/725 (83%)	544 (90%)	49 (8%)	8 (1%)	15	59
1	B	601/725 (83%)	544 (90%)	49 (8%)	8 (1%)	15	59
1	C	601/725 (83%)	543 (90%)	51 (8%)	7 (1%)	16	61
1	D	601/725 (83%)	543 (90%)	50 (8%)	8 (1%)	15	59
All	All	2404/2900 (83%)	2174 (90%)	199 (8%)	31 (1%)	15	59

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	449	ASP
1	B	17	VAL
1	B	449	ASP
1	C	17	VAL
1	C	449	ASP
1	D	17	VAL
1	D	449	ASP
1	A	114	TYR
1	A	194	ALA
1	B	114	TYR
1	B	194	ALA
1	C	114	TYR
1	C	194	ALA
1	D	114	TYR
1	D	194	ALA
1	A	345	SER
1	B	210	TYR
1	C	345	SER
1	B	345	SER
1	D	345	SER
1	B	40	LYS

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Mol	Chain	Res	Type
1	D	210	TYR
1	A	40	LYS
1	C	435	PRO
1	C	111	VAL
1	D	435	PRO
1	A	111	VAL
1	B	435	PRO
1	D	111	VAL
1	A	435	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	526/622 (85%)	481 (91%)	45 (9%)	13	49
1	B	526/622 (85%)	478 (91%)	48 (9%)	12	46
1	C	526/622 (85%)	479 (91%)	47 (9%)	12	47
1	D	526/622 (85%)	481 (91%)	45 (9%)	13	49
All	All	2104/2488 (85%)	1919 (91%)	185 (9%)	12	48

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	17	VAL
1	A	19	ASN
1	A	40	LYS
1	A	42	HIS
1	A	74	ARG
1	A	84	GLU
1	A	86	ARG
1	A	94	ARG
1	A	97	ILE
1	A	103	VAL
1	A	122	LEU

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	164	VAL
1	A	181	LYS
1	A	183	ARG
1	A	213	LEU
1	A	214	GLU
1	A	216	VAL
1	A	247	VAL
1	A	249	GLN
1	A	289	LYS
1	A	320	ARG
1	A	321	TYR
1	A	335	LEU
1	A	376	ARG
1	A	378	LEU
1	A	388	SER
1	A	399	ARG
1	A	428	ARG
1	A	458	LYS
1	A	459	ILE
1	A	469	SER
1	A	471	ARG
1	A	484	ASN
1	A	487	ILE
1	A	514	THR
1	A	525	SER
1	A	537	MET
1	A	552	TYR
1	A	556	ARG
1	A	568	LEU
1	A	596	LEU
1	A	633	SER
1	A	635	MET
1	B	7	ASN
1	B	17	VAL
1	B	19	ASN
1	B	40	LYS
1	B	42	HIS
1	B	74	ARG
1	B	84	GLU
1	B	86	ARG
1	B	94	ARG

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Mol	Chain	Res	Type
1	B	97	ILE
1	B	103	VAL
1	B	122	LEU
1	B	133	ASN
1	B	164	VAL
1	B	181	LYS
1	B	183	ARG
1	B	192	THR
1	B	213	LEU
1	B	214	GLU
1	B	216	VAL
1	B	247	VAL
1	B	249	GLN
1	B	289	LYS
1	B	320	ARG
1	B	321	TYR
1	B	335	LEU
1	B	376	ARG
1	B	378	LEU
1	B	388	SER
1	B	399	ARG
1	B	428	ARG
1	B	458	LYS
1	B	459	ILE
1	B	469	SER
1	B	471	ARG
1	B	484	ASN
1	B	487	ILE
1	B	513	TYR
1	B	514	THR
1	B	525	SER
1	B	537	MET
1	B	552	TYR
1	B	556	ARG
1	B	568	LEU
1	B	569	VAL
1	B	596	LEU
1	B	633	SER
1	B	635	MET
1	C	7	ASN
1	C	17	VAL
1	C	19	ASN

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Mol	Chain	Res	Type
1	C	40	LYS
1	C	42	HIS
1	C	74	ARG
1	C	84	GLU
1	C	86	ARG
1	C	94	ARG
1	C	97	ILE
1	C	103	VAL
1	C	122	LEU
1	C	133	ASN
1	C	164	VAL
1	C	181	LYS
1	C	183	ARG
1	C	192	THR
1	C	213	LEU
1	C	214	GLU
1	C	216	VAL
1	C	247	VAL
1	C	249	GLN
1	C	289	LYS
1	C	320	ARG
1	C	321	TYR
1	C	335	LEU
1	C	376	ARG
1	C	378	LEU
1	C	388	SER
1	C	399	ARG
1	C	428	ARG
1	C	458	LYS
1	C	459	ILE
1	C	469	SER
1	C	471	ARG
1	C	484	ASN
1	C	487	ILE
1	C	514	THR
1	C	525	SER
1	C	537	MET
1	C	552	TYR
1	C	556	ARG
1	C	568	LEU
1	C	569	VAL
1	C	596	LEU

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Mol	Chain	Res	Type
1	C	633	SER
1	C	635	MET
1	D	7	ASN
1	D	17	VAL
1	D	19	ASN
1	D	40	LYS
1	D	42	HIS
1	D	74	ARG
1	D	84	GLU
1	D	86	ARG
1	D	94	ARG
1	D	97	ILE
1	D	103	VAL
1	D	122	LEU
1	D	133	ASN
1	D	164	VAL
1	D	181	LYS
1	D	183	ARG
1	D	213	LEU
1	D	214	GLU
1	D	216	VAL
1	D	247	VAL
1	D	249	GLN
1	D	289	LYS
1	D	320	ARG
1	D	321	TYR
1	D	335	LEU
1	D	376	ARG
1	D	378	LEU
1	D	388	SER
1	D	399	ARG
1	D	428	ARG
1	D	458	LYS
1	D	459	ILE
1	D	469	SER
1	D	471	ARG
1	D	484	ASN
1	D	487	ILE
1	D	514	THR
1	D	525	SER
1	D	537	MET
1	D	552	TYR

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Mol	Chain	Res	Type
1	D	556	ARG
1	D	568	LEU
1	D	596	LEU
1	D	633	SER
1	D	635	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	78	HIS
1	A	133	ASN
1	A	168	HIS
1	A	239	HIS
1	A	300	HIS
1	A	484	ASN
1	A	500	HIS
1	A	621	GLN
1	B	6	GLN
1	B	78	HIS
1	B	133	ASN
1	B	168	HIS
1	B	239	HIS
1	B	300	HIS
1	B	484	ASN
1	B	500	HIS
1	B	621	GLN
1	C	6	GLN
1	C	78	HIS
1	C	133	ASN
1	C	168	HIS
1	C	239	HIS
1	C	300	HIS
1	C	484	ASN
1	C	500	HIS
1	C	621	GLN
1	D	6	GLN
1	D	78	HIS
1	D	133	ASN
1	D	168	HIS
1	D	239	HIS
1	D	300	HIS

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Mol	Chain	Res	Type
1	D	484	ASN
1	D	500	HIS
1	D	621	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	801	-	4,4,4	0.12	0	6,6,6	0.23	0
2	SO4	A	803	-	4,4,4	0.09	0	6,6,6	0.12	0
3	UDP	A	901	-	18,26,26	1.21	2 (11%)	26,40,40	1.65	4 (15%)
2	SO4	B	801	-	4,4,4	0.19	0	6,6,6	0.17	0
2	SO4	B	802	-	4,4,4	0.20	0	6,6,6	0.26	0
2	SO4	B	803	-	4,4,4	0.11	0	6,6,6	0.17	0
3	UDP	B	901	-	18,26,26	1.19	1 (5%)	26,40,40	1.58	2 (7%)
2	SO4	C	801	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	C	802	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	C	803	-	4,4,4	0.11	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UDP	C	901	-	18,26,26	1.12	1 (5%)	26,40,40	1.71	3 (11%)
2	SO4	D	801	-	4,4,4	0.09	0	6,6,6	0.22	0
2	SO4	D	802	-	4,4,4	0.28	0	6,6,6	0.24	0
2	SO4	D	803	-	4,4,4	0.19	0	6,6,6	0.43	0
3	UDP	D	901	-	18,26,26	1.07	1 (5%)	26,40,40	1.50	3 (11%)

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	801	-	-	0/0/0/0	0/0/0/0
2	SO4	A	803	-	-	0/0/0/0	0/0/0/0
3	UDP	A	901	-	-	0/12/32/32	0/2/2/2
2	SO4	B	801	-	-	0/0/0/0	0/0/0/0
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	B	803	-	-	0/0/0/0	0/0/0/0
3	UDP	B	901	-	-	0/12/32/32	0/2/2/2
2	SO4	C	801	-	-	0/0/0/0	0/0/0/0
2	SO4	C	802	-	-	0/0/0/0	0/0/0/0
2	SO4	C	803	-	-	0/0/0/0	0/0/0/0
3	UDP	C	901	-	-	0/12/32/32	0/2/2/2
2	SO4	D	801	-	-	0/0/0/0	0/0/0/0
2	SO4	D	802	-	-	0/0/0/0	0/0/0/0
2	SO4	D	803	-	-	0/0/0/0	0/0/0/0
3	UDP	D	901	-	-	0/12/32/32	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	UDP	O4'-C4'	-2.20	1.39	1.45
3	D	901	UDP	C4-N3	2.22	1.37	1.33
3	A	901	UDP	C4-N3	2.45	1.37	1.33
3	C	901	UDP	C4-N3	2.55	1.37	1.33
3	B	901	UDP	C4-N3	2.70	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	UDP	PA-O3A-PB	-4.35	118.09	132.67
3	D	901	UDP	PA-O3A-PB	-3.35	121.42	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	UDP	PA-O3A-PB	-2.99	122.65	132.67
3	A	901	UDP	PA-O3A-PB	-2.60	123.94	132.67
3	A	901	UDP	O3'-C3'-C4'	-2.26	104.27	111.05
3	A	901	UDP	C4'-O4'-C1'	2.13	112.06	109.72
3	C	901	UDP	C4'-O4'-C1'	2.20	112.14	109.72
3	D	901	UDP	C4'-O4'-C1'	2.25	112.19	109.72
3	D	901	UDP	C4-N3-C2	4.76	118.86	114.14
3	C	901	UDP	C4-N3-C2	5.69	119.78	114.14
3	B	901	UDP	C4-N3-C2	5.71	119.80	114.14
3	A	901	UDP	C4-N3-C2	6.02	120.10	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	UDP	2	0
2	B	801	SO4	1	0
3	B	901	UDP	2	0
3	C	901	UDP	4	0
2	D	801	SO4	1	0
3	D	901	UDP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	611/725 (84%)	-0.06	6 (0%) 84 76	45, 101, 130, 165	0
1	B	611/725 (84%)	-0.04	7 (1%) 82 74	49, 107, 135, 172	0
1	C	611/725 (84%)	-0.17	1 (0%) 95 93	45, 102, 130, 167	0
1	D	611/725 (84%)	-0.20	2 (0%) 94 91	39, 96, 125, 159	0
All	All	2444/2900 (84%)	-0.12	16 (0%) 89 83	39, 102, 132, 172	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	LEU	3.6
1	A	548	ASP	3.3
1	A	549	TYR	3.1
1	B	631	ASN	3.1
1	B	630	LEU	3.1
1	B	549	TYR	3.0
1	B	437	GLY	2.5
1	D	628	GLU	2.4
1	B	626	VAL	2.4
1	B	436	GLU	2.4
1	A	631	ASN	2.3
1	B	416	LEU	2.3
1	C	437	GLY	2.3
1	A	629	GLU	2.2
1	D	548	ASP	2.1
1	A	219	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	D	802	5/5	0.45	0.56	6.73	157,157,157,157	0
3	UDP	D	901	25/25	0.92	0.29	0.83	126,126,126,126	0
3	UDP	C	901	25/25	0.91	0.26	0.79	133,133,133,133	0
3	UDP	B	901	25/25	0.91	0.28	0.31	109,109,109,109	0
3	UDP	A	901	25/25	0.93	0.27	-0.30	104,104,104,104	0
2	SO4	D	803	5/5	0.90	0.22	-0.42	138,138,138,138	0
2	SO4	A	803	5/5	0.87	0.24	-0.70	143,143,143,143	0
2	SO4	C	802	5/5	0.78	0.38	-	162,162,162,162	0
2	SO4	A	801	5/5	0.86	0.31	-	133,133,133,133	0
2	SO4	B	803	5/5	0.84	0.26	-	164,164,164,164	0
2	SO4	B	801	5/5	0.86	0.36	-	133,133,133,133	0
2	SO4	C	801	5/5	0.90	0.21	-	131,131,131,131	0
2	SO4	B	802	5/5	0.78	0.29	-	145,145,145,145	0
2	SO4	D	801	5/5	0.94	0.14	-	126,126,126,126	0
2	SO4	C	803	5/5	0.89	0.27	-	156,156,156,156	0

6.5 Other polymers [i](#)

There are no such residues in this entry.