



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:29 am BST

PDB ID : 3NCH
Title : Yeast Glycogen Synthase (Gsy2p) Basal State Conformation
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2010-06-04
Resolution : 2.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

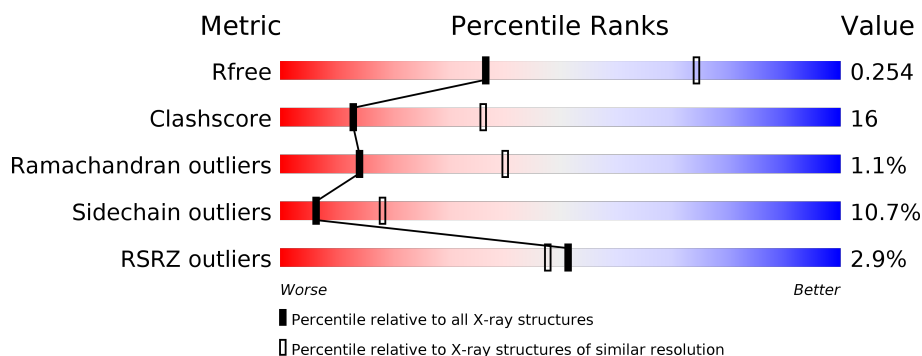
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	725	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>27%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	725	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>28%</div> <div>5%</div> <div>16%</div> </div> </div>
1	C	725	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>22%</div> <div>5%</div> <div>15%</div> </div> </div>
1	D	725	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>23%</div> <div>•</div> <div>16%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19787 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	612	Total	C	N	O	S	0	0	0
			4927	3150	858	900	19			
1	C	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			
1	D	612	Total	C	N	O	S	0	0	0
			4927	3150	858	900	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	A	1	Total	O	S	0	0
			5	4	1		
2	A	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	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	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		

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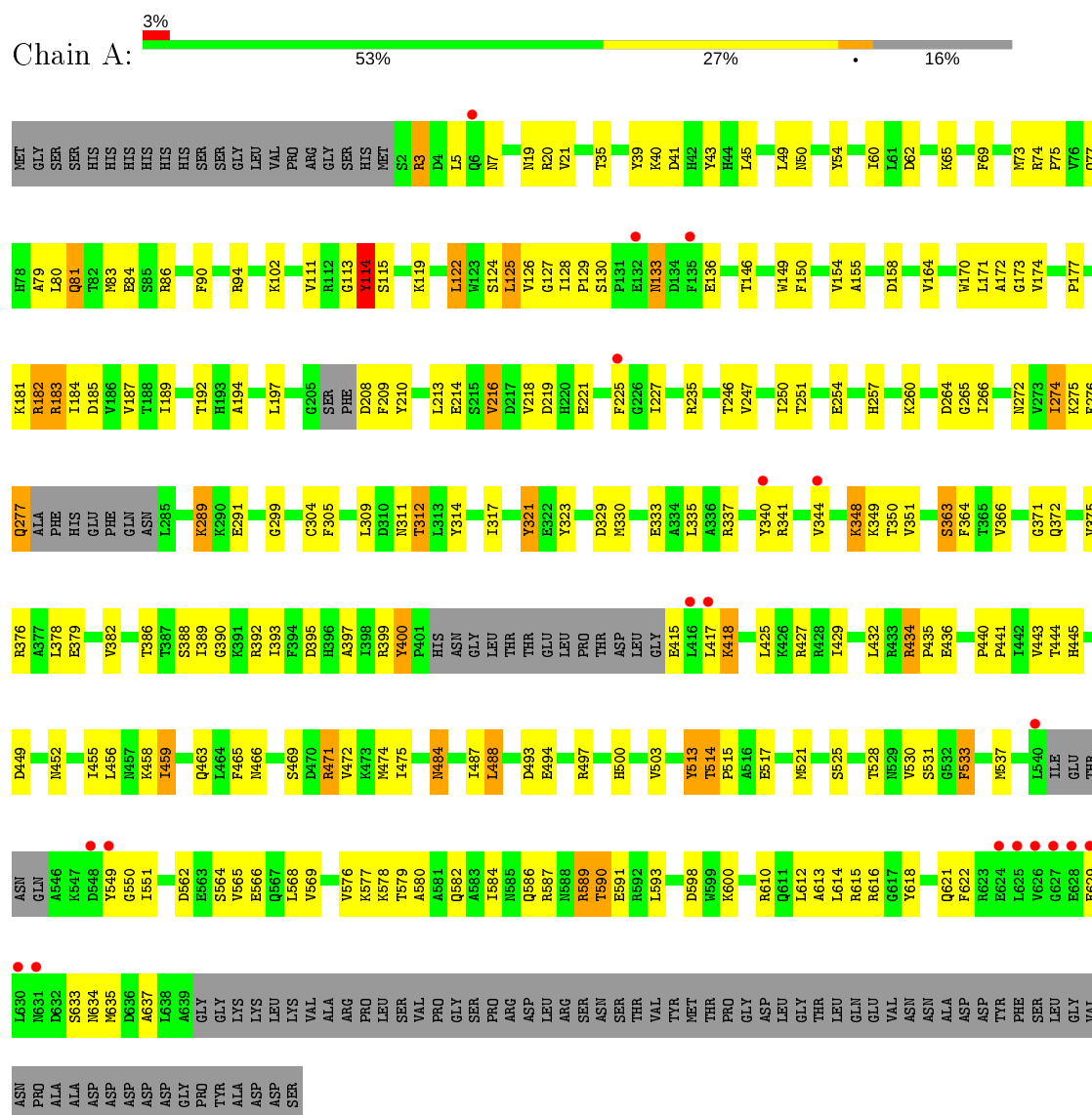
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots [i](#)

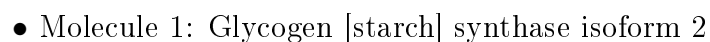
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

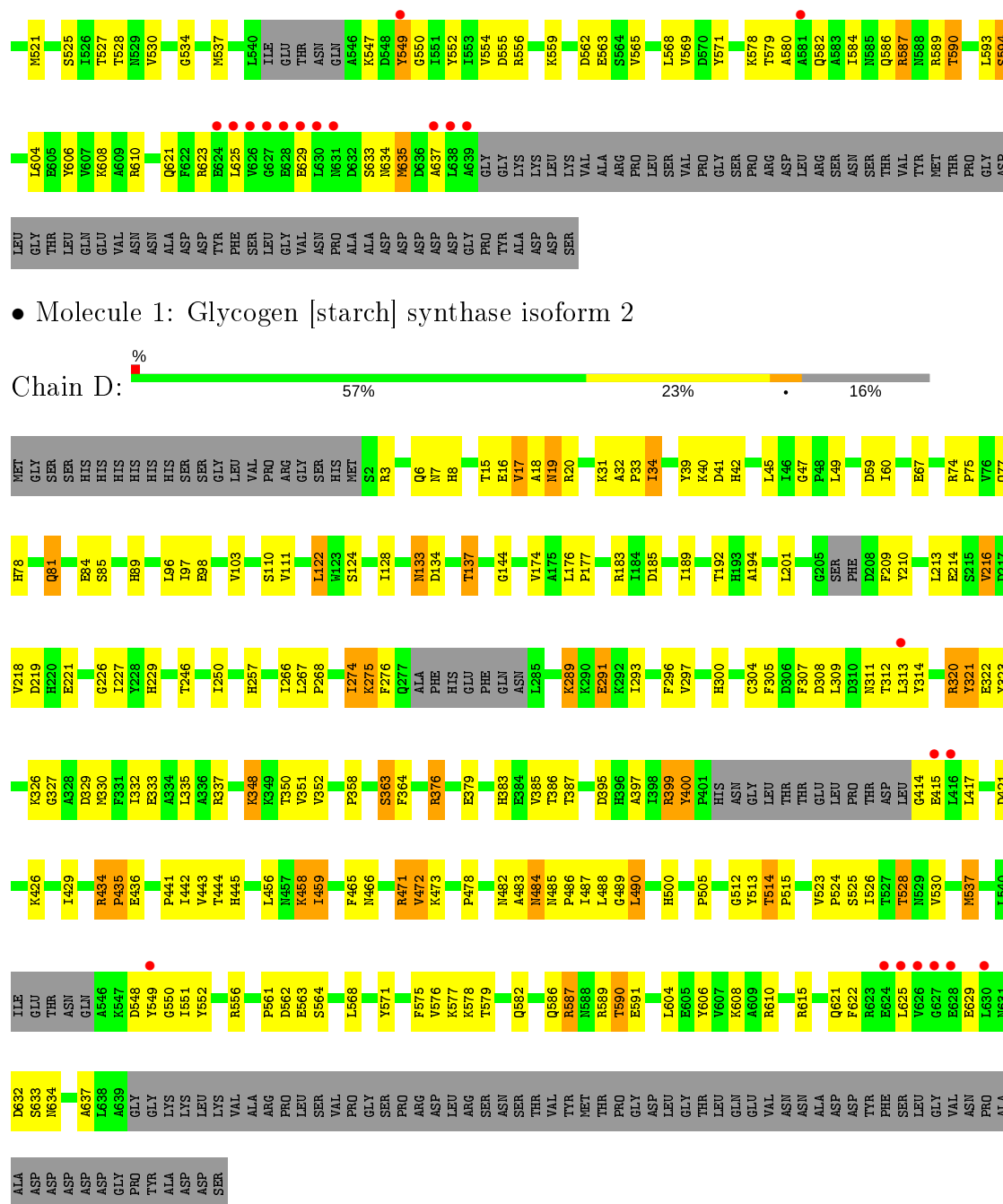


- Molecule 1: Glycogen [starch] synthase isoform 2





LEU	G414	E322	L213	L61	MET
	G415	Y323	E214	D62	GLY
L416	E415	K326	V216	K65	SER
	L417			P66	HIS
K418	S419	M330	E221	E72	HIS
S419		F331	I227		
L425	L425	I332	I227	R74	HIS
K426	L426	L335	R230	P75	SER
I429	K434	Y340	E234	V76	SER
		V344	T246	Q77	GLY
P435	P435	V344	A79	L30	LEU
E436	E436	S345	L259	Q81	VAL
P440	P441	G346	D264	T82	PRO
		S347		M83	ARG
I442	K348	K348	G265	T83	GLY
V443	V443	T350	I266	S85	SER
	V443	T350	L267	S85	HIS
L456	K457	V351	P268	L96	MET
		F354	L271	V111	S2
K468	I459	A359	Q277	L122	R3
R460	R460	S363	ALA	L128	Q6
V462	V462	F364	PHE	N133	N7
Q463	Q463	Q372	GLU	E136	F10
L464	L464	F465	PHE		F11
F465	F465	R376	GLN	T15	E12
S469	S469	D470	N284	D158	T13
D472	D472	H383	H286	E16	A14
K471	K471	T386	K289	T163	T15
V472	V472	T387	K290	H168	E16
M474	M474	G390	E291	L176	V17
E479	F480	F394	F296	P177	A18
			H396	K181	N19
N481	N481	D395	F301	R182	K31
N482	N482	H397	H302	R183	A32
P486	P486	I398	F305	I184	P33
I487	I487	R399	D306	D185	I34
L488	L488	Y400	F307	V186	T35
G489	G489	P401	D308	I189	V36
L490	L490	HIS	L309		K40
D493	D493	ASN	D310	D41	D41
V496	H500	GLY	N311	T192	H42
		LEU	T312	Y43	H43
H500	Y513	THR	L313	R199	H44
		THR	Y314	G205	L45
P496	P496	GLU	F315	PHE	I46
H500	H500	LEU	F316	THR	G47
Y513	Y513	PRO	R320	D208	D59
T514	T514	THR	K223	L208	L60
L515	L515	ASP			



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.94Å 161.84Å 121.62Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	46.73 – 2.88 46.73 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.73-2.88) 98.3 (46.73-2.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.213 , 0.265 0.206 , 0.254	Depositor DCC
R_{free} test set	4043 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19787	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/5038	0.59	0/6819
1	B	0.44	0/5042	0.58	0/6824
1	C	0.41	0/5050	0.58	0/6835
1	D	0.43	0/5042	0.58	0/6824
All	All	0.43	0/20172	0.58	0/27302

There are no bond length outliers.

There are no bond angle outliers.

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	171	0
1	B	4927	0	4853	182	0
1	C	4935	0	4859	148	0
1	D	4927	0	4853	155	0
2	A	20	0	0	1	0
2	B	15	0	0	1	0
2	C	20	0	0	0	0
2	D	20	0	0	1	0
All	All	19787	0	19415	642	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 (642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:THR:HG22	1:B:350:THR:HB	1.15	1.13
1:B:125:LEU:HD21	1:B:181:LYS:HG3	1.40	1.04
1:B:382:VAL:O	1:B:386:THR:HG23	1.58	1.03
1:B:493:ASP:HB2	1:B:521:MET:HE2	1.40	1.02
1:A:589:ARG:HG3	1:A:589:ARG:HH11	1.21	1.00
1:A:312:THR:CG2	1:A:350:THR:HB	1.92	0.99
1:D:314:TYR:H	1:D:500:HIS:HD2	1.07	0.99
1:A:351:VAL:HB	1:A:472:VAL:HG12	1.44	0.97
1:A:133:ASN:H	1:A:133:ASN:HD22	1.14	0.95
1:A:299:GLY:HA2	1:A:375:VAL:HG21	1.51	0.93
1:D:312:THR:HG22	1:D:350:THR:HB	1.50	0.92
1:C:314:TYR:H	1:C:500:HIS:HD2	1.16	0.92
1:C:589:ARG:HG3	1:C:589:ARG:HH11	1.33	0.92
1:B:312:THR:CG2	1:B:350:THR:HB	1.99	0.91
1:A:312:THR:HG22	1:A:350:THR:HB	1.50	0.90
1:C:312:THR:HG22	1:C:350:THR:HB	1.53	0.90
1:C:133:ASN:HD22	1:C:133:ASN:H	1.20	0.89
1:A:125:LEU:HD21	1:A:181:LYS:HG3	1.53	0.89
1:B:493:ASP:HB2	1:B:521:MET:CE	2.04	0.87
1:C:493:ASP:HB2	1:C:521:MET:HE1	1.59	0.85
1:B:585:ASN:HB3	1:B:589:ARG:HH12	1.42	0.83
1:A:348:LYS:HE2	1:A:349:LYS:HE2	1.60	0.83
1:C:549:TYR:CD2	1:C:589:ARG:HB3	2.14	0.83
1:A:528:THR:HG22	1:A:530:VAL:H	1.44	0.82
1:D:122:LEU:HD13	1:D:128:ILE:HB	1.61	0.82
1:B:122:LEU:HD13	1:B:128:ILE:HB	1.61	0.81
1:A:390:GLY:HA2	1:C:386:THR:HG21	1.63	0.81
1:C:528:THR:HG22	1:C:530:VAL:H	1.44	0.80
1:A:309:LEU:HA	1:A:312:THR:OG1	1.80	0.79
1:D:74:ARG:HH21	1:D:77:GLN:HE22	1.29	0.79
1:A:122:LEU:HD13	1:A:128:ILE:HB	1.63	0.79
1:C:549:TYR:O	1:C:590:THR:HG22	1.83	0.79
1:A:62:ASP:OD2	1:A:65:LYS:HG3	1.83	0.78
1:A:314:TYR:H	1:A:500:HIS:HD2	1.32	0.78
1:D:589:ARG:HH11	1:D:589:ARG:HG3	1.47	0.78
1:C:579:THR:OG1	1:C:582:GLN:HG3	1.85	0.77
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ASN:H	1:B:484:ASN:HD22	1.31	0.76
1:A:133:ASN:ND2	1:A:133:ASN:H	1.82	0.76
1:C:434:ARG:NH2	1:C:440:PRO:HA	2.00	0.76
1:A:75:PRO:HG2	1:A:158:ASP:OD2	1.86	0.76
1:B:551:ILE:HD12	1:B:593:LEU:HD13	1.68	0.76
1:B:390:GLY:HA2	1:D:386:THR:HG21	1.68	0.75
1:A:81:GLN:HE21	1:A:81:GLN:HA	1.51	0.75
1:C:549:TYR:HD2	1:C:589:ARG:HB3	1.47	0.75
1:B:549:TYR:CE2	1:B:589:ARG:HD3	2.22	0.75
1:B:528:THR:HG22	1:B:530:VAL:H	1.52	0.74
1:C:434:ARG:HH21	1:C:440:PRO:HA	1.51	0.74
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.18	0.74
1:C:6:GLN:NE2	1:C:625:LEU:HD21	2.03	0.74
1:B:589:ARG:HH11	1:B:589:ARG:HG3	1.52	0.73
1:D:214:GLU:HG2	1:D:257:HIS:CE1	2.23	0.73
1:B:174:VAL:O	1:B:177:PRO:HD2	1.88	0.72
1:C:74:ARG:HE	1:C:77:GLN:NE2	1.87	0.72
1:D:214:GLU:HG2	1:D:257:HIS:ND1	2.05	0.72
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.54	0.71
1:A:289:LYS:HG2	1:A:494:GLU:HB3	1.71	0.71
1:D:549:TYR:O	1:D:590:THR:HG22	1.90	0.71
1:B:75:PRO:HG2	1:B:158:ASP:OD2	1.89	0.71
1:A:382:VAL:O	1:A:386:THR:HG23	1.90	0.71
1:D:133:ASN:HD22	1:D:133:ASN:H	1.39	0.70
1:A:589:ARG:NH1	1:A:589:ARG:HG3	2.01	0.70
1:B:445:HIS:CD2	1:B:478:PRO:HD2	2.26	0.70
1:C:286:HIS:HB2	1:C:587:ARG:HH12	1.56	0.70
1:C:589:ARG:HG3	1:C:589:ARG:NH1	2.04	0.70
1:A:390:GLY:CA	1:C:386:THR:HG21	2.20	0.70
1:C:399:ARG:O	1:C:400:TYR:C	2.30	0.70
1:B:80:LEU:HD22	1:B:90:PHE:CE1	2.27	0.69
1:A:111:VAL:O	1:A:111:VAL:HG12	1.92	0.69
1:D:314:TYR:H	1:D:500:HIS:CD2	2.00	0.69
1:D:383:HIS:O	1:D:387:THR:HG23	1.92	0.69
1:B:80:LEU:HB3	1:B:90:PHE:CZ	2.28	0.68
1:C:32:ALA:HB3	1:C:33:PRO:HD3	1.75	0.68
1:C:443:VAL:HG22	1:C:456:LEU:HD21	1.76	0.67
1:A:314:TYR:H	1:A:500:HIS:CD2	2.12	0.67
1:B:484:ASN:HD22	1:B:484:ASN:N	1.93	0.67
1:A:5:LEU:HD21	1:A:618:TYR:HD1	1.59	0.67
1:B:125:LEU:HD21	1:B:181:LYS:CG	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ARG:HH21	1:B:260:LYS:HG3	1.60	0.67
1:B:125:LEU:CD2	1:B:181:LYS:HG3	2.23	0.66
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.30	0.66
1:C:314:TYR:H	1:C:500:HIS:CD2	2.05	0.66
1:A:493:ASP:HB2	1:A:521:MET:CE	2.26	0.66
1:D:122:LEU:CD1	1:D:128:ILE:HB	2.25	0.66
1:D:615:ARG:HD3	1:D:622:PHE:CD1	2.31	0.66
1:C:286:HIS:HB2	1:C:587:ARG:NH1	2.11	0.65
1:D:6:GLN:NE2	1:D:625:LEU:HD21	2.11	0.65
1:B:549:TYR:O	1:B:590:THR:HG22	1.97	0.65
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.62	0.65
1:D:74:ARG:HE	1:D:77:GLN:NE2	1.94	0.65
1:A:449:ASP:OD2	1:A:452:ASN:HB2	1.97	0.65
1:A:312:THR:HG23	1:A:350:THR:HB	1.75	0.65
1:C:133:ASN:HD22	1:C:133:ASN:N	1.90	0.65
1:C:383:HIS:O	1:C:387:THR:HG23	1.97	0.64
1:B:143:LEU:O	1:B:147:VAL:HG23	1.97	0.64
1:B:314:TYR:H	1:B:500:HIS:CD2	2.16	0.64
1:B:309:LEU:HA	1:B:312:THR:OG1	1.96	0.64
1:D:550:GLY:HA3	1:D:590:THR:HG21	1.80	0.64
1:C:634:ASN:HB2	1:C:637:ALA:H	1.62	0.63
1:A:305:PHE:HZ	1:A:309:LEU:HG	1.62	0.63
1:B:133:ASN:H	1:B:133:ASN:ND2	1.97	0.63
1:C:227:ILE:HG22	1:C:227:ILE:O	1.99	0.63
1:A:589:ARG:HH11	1:A:589:ARG:CG	2.02	0.63
1:D:483:ALA:HA	1:D:490:LEU:N	2.14	0.63
1:A:340:TYR:CE2	1:A:344:VAL:HG21	2.34	0.63
1:B:484:ASN:ND2	1:B:484:ASN:H	1.97	0.63
1:A:125:LEU:HD21	1:A:181:LYS:CG	2.27	0.62
1:B:340:TYR:CE2	1:B:344:VAL:HG21	2.35	0.62
1:B:351:VAL:HB	1:B:472:VAL:CG1	2.29	0.62
1:D:216:VAL:HG23	1:D:221:GLU:HG3	1.80	0.62
1:D:589:ARG:NH1	1:D:589:ARG:HG3	2.15	0.62
1:D:550:GLY:HA3	1:D:590:THR:HG22	1.82	0.62
1:A:579:THR:HG23	1:A:582:GLN:OE1	1.99	0.62
1:B:348:LYS:HE2	1:B:349:LYS:HE2	1.82	0.61
1:B:213:LEU:HD11	1:B:253:PHE:CE1	2.35	0.61
1:D:444:THR:OG1	1:D:445:HIS:HD2	1.82	0.61
1:C:17:VAL:HG23	1:C:18:ALA:H	1.65	0.61
1:C:307:PHE:HD1	1:C:312:THR:HG21	1.65	0.61
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:ASN:HB2	1:D:637:ALA:H	1.65	0.61
1:A:444:THR:OG1	1:A:445:HIS:HD2	1.83	0.61
1:D:323:TYR:CE1	1:D:329:ASP:HB3	2.35	0.61
1:A:122:LEU:CD1	1:A:128:ILE:HB	2.30	0.61
1:C:493:ASP:HB2	1:C:521:MET:CE	2.29	0.61
1:A:493:ASP:HB2	1:A:521:MET:HE2	1.81	0.60
1:C:133:ASN:ND2	1:C:133:ASN:H	1.97	0.60
1:A:5:LEU:HD21	1:A:618:TYR:CD1	2.36	0.60
1:C:340:TYR:CE2	1:C:344:VAL:HG21	2.36	0.60
1:D:385:VAL:HG22	1:D:421:ASP:HB3	1.82	0.60
1:B:390:GLY:CA	1:D:386:THR:HG21	2.30	0.60
1:B:548:ASP:O	1:B:589:ARG:HD2	2.02	0.60
1:B:549:TYR:HB3	1:B:593:LEU:HD11	1.82	0.60
1:C:234:GLU:HG2	1:C:259:LEU:HD21	1.82	0.60
1:B:133:ASN:HD22	1:B:133:ASN:H	1.50	0.60
1:A:528:THR:CG2	1:A:530:VAL:HG22	2.32	0.59
1:C:216:VAL:HG23	1:C:221:GLU:HG3	1.83	0.59
1:B:623:ARG:HE	1:B:629:GLU:HB3	1.67	0.59
1:D:307:PHE:CD1	1:D:312:THR:HG21	2.37	0.59
1:A:634:ASN:HB2	1:A:637:ALA:H	1.67	0.59
1:B:620:ASP:O	1:B:624:GLU:HG2	2.03	0.59
1:A:309:LEU:HA	1:A:312:THR:HG1	1.67	0.59
1:D:275:LYS:O	1:D:275:LYS:HG2	2.03	0.59
1:A:289:LYS:CG	1:A:494:GLU:HB3	2.33	0.59
1:D:548:ASP:O	1:D:589:ARG:HD2	2.03	0.59
1:B:327:GLY:HA3	1:B:505:PRO:O	2.03	0.58
1:D:89:HIS:HD2	1:D:110:SER:HB2	1.67	0.58
1:A:111:VAL:O	1:A:111:VAL:CG1	2.51	0.58
1:B:266:ILE:HG22	1:B:268:PRO:HG3	1.85	0.58
1:C:332:ILE:HG12	1:C:474:MET:HE2	1.84	0.58
1:A:213:LEU:HD12	1:A:214:GLU:N	2.18	0.58
1:B:323:TYR:OH	1:B:458:LYS:HG3	2.02	0.58
1:B:606:TYR:O	1:B:610:ARG:HG3	2.03	0.58
1:B:414:GLY:HA2	1:D:414:GLY:N	2.18	0.58
1:C:17:VAL:HG23	1:C:18:ALA:N	2.17	0.58
1:C:266:ILE:HG22	1:C:268:PRO:HD3	1.85	0.58
1:C:21:VAL:HG12	1:C:21:VAL:O	2.03	0.58
1:D:445:HIS:CD2	1:D:478:PRO:HD2	2.38	0.58
1:C:307:PHE:CD1	1:C:312:THR:HG21	2.38	0.57
1:D:67:GLU:CD	1:D:67:GLU:H	2.07	0.57
1:B:11:PHE:HD1	1:B:46:ILE:HD11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ARG:HD3	1:A:622:PHE:CD1	2.40	0.57
1:B:589:ARG:HG3	1:B:589:ARG:NH1	2.19	0.57
1:C:552:TYR:HD1	1:C:571:TYR:CD2	2.22	0.57
1:D:45:LEU:HB2	1:D:103:VAL:HG12	1.86	0.57
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.87	0.57
1:D:17:VAL:HG23	1:D:18:ALA:H	1.70	0.57
1:D:308:ASP:O	1:D:312:THR:HG23	2.04	0.57
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.37	0.57
1:D:17:VAL:HG22	1:D:47:GLY:HA3	1.87	0.57
1:B:399:ARG:NH2	1:D:308:ASP:HA	2.20	0.57
1:D:305:PHE:HZ	1:D:309:LEU:HG	1.69	0.57
1:A:375:VAL:O	1:A:379:GLU:HG3	2.05	0.56
1:A:225:PHE:O	1:A:227:ILE:HG12	2.05	0.56
1:B:235:ARG:NH2	1:B:260:LYS:HG3	2.19	0.56
1:B:271:LEU:HD13	1:B:520:VAL:HG21	1.87	0.56
1:C:425:LEU:O	1:C:429:ILE:HG13	2.05	0.56
1:D:81:GLN:CA	1:D:81:GLN:HE21	2.19	0.56
1:B:307:PHE:CD1	1:B:312:THR:HG21	2.39	0.56
1:D:484:ASN:H	1:D:484:ASN:ND2	2.03	0.56
1:B:74:ARG:HE	1:B:77:GLN:NE2	2.04	0.56
1:C:213:LEU:HA	1:C:216:VAL:CG1	2.36	0.56
1:D:216:VAL:CG2	1:D:221:GLU:HG3	2.36	0.56
1:B:89:HIS:O	1:B:107:ASP:HB3	2.06	0.56
1:D:314:TYR:N	1:D:500:HIS:HD2	1.90	0.56
1:A:119:LYS:HB3	1:A:130:SER:OG	2.05	0.56
1:A:181:LYS:C	1:A:183:ARG:H	2.09	0.56
1:C:308:ASP:O	1:C:312:THR:HG23	2.06	0.56
1:B:579:THR:HG23	1:B:582:GLN:OE1	2.05	0.56
1:C:443:VAL:CG2	1:C:456:LEU:HD21	2.36	0.56
1:D:358:PRO:HA	1:D:478:PRO:O	2.06	0.56
1:D:3:ARG:HH12	1:D:185:ASP:HB3	1.71	0.56
1:A:434:ARG:NH2	1:A:440:PRO:HA	2.21	0.55
1:D:174:VAL:O	1:D:177:PRO:HD2	2.06	0.55
1:A:79:ALA:O	1:A:83:MET:HG2	2.06	0.55
1:D:213:LEU:HD12	1:D:214:GLU:N	2.21	0.55
1:A:218:VAL:HG23	1:A:219:ASP:N	2.21	0.55
1:C:234:GLU:HG2	1:C:259:LEU:CD2	2.37	0.55
1:A:350:THR:OG1	1:A:471:ARG:NH1	2.36	0.55
1:B:210:TYR:CZ	1:B:530:VAL:HB	2.41	0.55
1:D:31:LYS:HE2	1:D:606:TYR:CE1	2.41	0.55
1:B:463:GLN:HG2	1:B:465:PHE:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASP:OD2	1:B:65:LYS:HG3	2.07	0.55
1:C:350:THR:OG1	1:C:471:ARG:NH1	2.37	0.55
1:D:483:ALA:HA	1:D:490:LEU:H	1.70	0.55
1:A:379:GLU:HG2	1:C:394:PHE:CE1	2.42	0.55
1:A:565:VAL:O	1:A:569:VAL:HG23	2.07	0.55
1:D:213:LEU:HA	1:D:216:VAL:CG1	2.37	0.55
1:B:528:THR:CG2	1:B:530:VAL:HG22	2.36	0.54
1:B:493:ASP:CB	1:B:521:MET:HE2	2.25	0.54
1:D:19:ASN:HD22	1:D:19:ASN:N	2.05	0.54
1:D:528:THR:HG22	1:D:530:VAL:H	1.73	0.54
1:D:579:THR:OG1	1:D:582:GLN:HG3	2.07	0.54
1:D:134:ASP:OD2	1:D:229:HIS:NE2	2.39	0.54
1:D:17:VAL:CG2	1:D:47:GLY:HA3	2.37	0.54
1:D:332:ILE:HD13	1:D:459:ILE:HG23	1.90	0.54
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.90	0.54
1:C:82:THR:O	1:C:85:SER:HB2	2.08	0.54
1:D:274:ILE:O	1:D:276:PHE:N	2.34	0.54
1:A:146:THR:O	1:A:149:TRP:HB3	2.08	0.54
1:A:487:ILE:HG22	1:A:488:LEU:N	2.22	0.54
1:B:449:ASP:OD2	1:B:452:ASN:HB2	2.07	0.54
1:C:31:LYS:O	1:C:35:THR:HG23	2.08	0.54
1:C:81:GLN:CA	1:C:81:GLN:HE21	2.20	0.54
1:B:227:ILE:HG22	1:B:227:ILE:O	2.06	0.53
1:B:444:THR:OG1	1:B:445:HIS:HD2	1.91	0.53
1:B:549:TYR:CD2	1:B:589:ARG:HD3	2.42	0.53
1:D:333:GLU:HG3	1:D:337:ARG:HH11	1.73	0.53
1:D:526:ILE:HG12	1:D:552:TYR:HB2	1.90	0.53
1:B:8:HIS:CE1	1:B:39:TYR:HE1	2.26	0.53
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.42	0.53
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.91	0.53
1:C:216:VAL:CG2	1:C:221:GLU:HG3	2.38	0.53
1:A:235:ARG:HH21	1:A:260:LYS:HG3	1.74	0.53
1:B:317:ILE:HG13	1:B:503:VAL:O	2.09	0.53
1:C:554:VAL:HG12	1:C:555:ASP:N	2.24	0.53
1:C:586:GLN:O	1:C:590:THR:HG23	2.09	0.53
1:B:314:TYR:H	1:B:500:HIS:HD2	1.52	0.53
1:B:332:ILE:HD13	1:B:459:ILE:HG23	1.90	0.53
1:A:39:TYR:HB2	1:A:43:TYR:HB2	1.90	0.53
1:B:351:VAL:HB	1:B:472:VAL:HG13	1.90	0.53
1:B:465:PHE:O	1:B:466:ASN:HB2	2.09	0.53
1:C:176:LEU:HB2	1:C:177:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:O	1:B:224:ARG:HB3	2.10	0.52
1:C:302:HIS:O	1:C:302:HIS:CG	2.62	0.52
1:D:442:ILE:HD12	1:D:459:ILE:HG13	1.91	0.52
1:A:371:GLY:O	1:A:375:VAL:HG23	2.09	0.52
1:B:150:PHE:O	1:B:154:VAL:HG23	2.08	0.52
1:A:341:ARG:NH2	1:A:566:GLU:OE1	2.42	0.52
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.39	0.52
1:B:585:ASN:HB3	1:B:589:ARG:NH1	2.19	0.52
1:D:274:ILE:C	1:D:276:PHE:H	2.11	0.52
1:A:49:LEU:HD11	1:A:54:TYR:CG	2.44	0.52
1:A:443:VAL:HG22	1:A:456:LEU:HD21	1.91	0.52
1:A:20:ARG:NH1	2:A:802:SO4:O3	2.26	0.52
1:A:187:VAL:HG21	1:A:614:LEU:HD23	1.91	0.52
1:A:372:GLN:HG3	1:A:487:ILE:HG12	1.92	0.52
1:B:259:LEU:O	1:B:260:LYS:HB2	2.10	0.52
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.40	0.52
1:A:174:VAL:O	1:A:177:PRO:HD2	2.10	0.52
1:A:264:ASP:O	1:A:635:MET:HG3	2.09	0.52
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.75	0.52
1:B:114:TYR:HD1	1:B:114:TYR:H	1.56	0.52
1:A:386:THR:HG21	1:C:390:GLY:HA2	1.91	0.52
1:A:586:GLN:O	1:A:590:THR:HG23	2.11	0.52
1:B:8:HIS:HE1	1:B:39:TYR:CE1	2.28	0.52
1:D:528:THR:CG2	1:D:530:VAL:H	2.23	0.52
1:A:213:LEU:HA	1:A:216:VAL:HG12	1.91	0.51
1:C:122:LEU:HD13	1:C:128:ILE:HB	1.91	0.51
1:C:66:PRO:O	1:C:74:ARG:NH2	2.43	0.51
1:D:266:ILE:HG22	1:D:268:PRO:HD3	1.91	0.51
1:A:311:ASN:HD21	1:A:348:LYS:HD2	1.75	0.51
1:B:586:GLN:O	1:B:590:THR:HG23	2.08	0.51
1:B:20:ARG:NH1	2:B:802:SO4:O2	2.34	0.51
1:C:265:GLY:HA3	1:C:635:MET:HG3	1.93	0.51
1:A:549:TYR:HB3	1:A:593:LEU:HD11	1.92	0.51
1:B:383:HIS:O	1:B:387:THR:HG23	2.11	0.51
1:A:192:THR:HG22	1:A:246:THR:HG22	1.92	0.51
1:B:351:VAL:HB	1:B:472:VAL:HG12	1.92	0.51
1:C:74:ARG:HH21	1:C:77:GLN:HE22	1.58	0.51
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.91	0.51
1:A:317:ILE:HG13	1:A:503:VAL:O	2.11	0.51
1:B:213:LEU:HA	1:B:216:VAL:CG1	2.40	0.51
1:C:580:ALA:O	1:C:584:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:THR:HG22	1:D:246:THR:HG22	1.93	0.51
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.46	0.51
1:A:528:THR:HG21	1:A:530:VAL:HG22	1.93	0.51
1:B:79:ALA:O	1:B:83:MET:HG2	2.11	0.51
1:C:623:ARG:HE	1:C:629:GLU:HB3	1.76	0.51
1:D:227:ILE:HG22	1:D:227:ILE:O	2.11	0.51
1:A:81:GLN:HE21	1:A:81:GLN:CA	2.22	0.51
1:B:493:ASP:CB	1:B:521:MET:CE	2.82	0.51
1:B:634:ASN:HB2	1:B:637:ALA:H	1.76	0.51
1:B:400:TYR:CG	1:B:401:PRO:HA	2.45	0.50
1:D:307:PHE:HD1	1:D:312:THR:HG21	1.75	0.50
1:B:423:VAL:HG12	1:B:424:MET:N	2.25	0.50
1:B:17:VAL:HG23	1:B:18:ALA:N	2.27	0.50
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.93	0.50
1:B:17:VAL:O	1:B:95:TRP:CZ2	2.64	0.50
1:A:170:TRP:O	1:A:173:GLY:N	2.42	0.50
1:A:21:VAL:CG1	1:A:21:VAL:O	2.59	0.50
1:B:94:ARG:HD3	1:B:100:ALA:HB1	1.92	0.50
1:B:113:GLY:C	1:B:115:SER:H	2.15	0.50
1:B:350:THR:OG1	1:B:471:ARG:NH1	2.34	0.50
1:C:330:MET:HE2	1:C:568:LEU:HD22	1.93	0.50
1:D:586:GLN:O	1:D:590:THR:HG23	2.12	0.50
1:A:235:ARG:NH2	1:A:260:LYS:HG3	2.27	0.50
1:B:501:LEU:HD12	1:B:524:PRO:HB2	1.94	0.50
1:C:17:VAL:HG22	1:C:47:GLY:HA3	1.93	0.50
1:D:267:LEU:HD22	1:D:606:TYR:CD2	2.47	0.50
1:A:276:PHE:O	1:A:277:GLN:HG3	2.12	0.49
1:A:576:VAL:C	1:A:578:LYS:H	2.14	0.49
1:C:442:ILE:HD12	1:C:459:ILE:HG13	1.94	0.49
1:A:415:GLU:HG2	1:A:417:LEU:O	2.13	0.49
1:A:73:MET:C	1:A:75:PRO:HD2	2.32	0.49
1:B:126:VAL:HB	1:B:128:ILE:HD12	1.94	0.49
1:B:506:SER:O	1:B:528:THR:HG21	2.11	0.49
1:B:425:LEU:O	1:B:429:ILE:HG13	2.12	0.49
1:A:213:LEU:C	1:A:213:LEU:HD12	2.33	0.49
1:A:39:TYR:CB	1:A:43:TYR:HB2	2.41	0.49
1:A:580:ALA:O	1:A:584:ILE:HG13	2.12	0.49
1:C:463:GLN:HG2	1:C:465:PHE:HE2	1.77	0.49
1:A:216:VAL:CG2	1:A:221:GLU:HG3	2.43	0.49
1:D:74:ARG:HE	1:D:77:GLN:HE21	1.60	0.49
1:B:126:VAL:HB	1:B:128:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE1	1:A:250:ILE:HD11	2.47	0.49
1:C:320:ARG:O	1:C:322:GLU:N	2.44	0.49
1:D:352:VAL:HG22	1:D:473:LYS:HB2	1.95	0.49
1:A:378:LEU:HD22	1:A:432:LEU:HD11	1.95	0.49
1:C:267:LEU:HD22	1:C:606:TYR:CD2	2.48	0.49
1:C:31:LYS:HZ3	1:C:35:THR:HG21	1.78	0.49
1:A:21:VAL:HG12	1:A:21:VAL:O	2.12	0.48
1:D:489:GLY:O	1:D:490:LEU:HG	2.13	0.48
1:B:434:ARG:HD2	1:B:435:PRO:HD2	1.93	0.48
1:D:6:GLN:HE21	1:D:625:LEU:HD21	1.77	0.48
1:A:351:VAL:CB	1:A:472:VAL:HG12	2.30	0.48
1:D:20:ARG:NH1	2:D:802:SO4:O3	2.45	0.48
1:A:276:PHE:O	1:A:497:ARG:NH2	2.46	0.48
1:C:549:TYR:HE2	1:C:589:ARG:HG2	1.78	0.48
1:D:512:GLY:O	1:D:515:PRO:HD2	2.13	0.48
1:A:125:LEU:CD2	1:A:181:LYS:HG3	2.34	0.48
1:B:551:ILE:HD12	1:B:593:LEU:CD1	2.39	0.48
1:A:598:ASP:OD2	1:A:600:LYS:HG3	2.12	0.48
1:B:31:LYS:O	1:B:35:THR:HG23	2.14	0.48
1:D:266:ILE:HG22	1:D:268:PRO:HG3	1.96	0.48
1:D:289:LYS:HD2	1:D:289:LYS:N	2.27	0.48
1:A:214:GLU:HG2	1:A:257:HIS:CE1	2.49	0.48
1:C:213:LEU:C	1:C:213:LEU:HD12	2.34	0.48
1:A:182:ARG:HB2	1:A:184:ILE:HG13	1.95	0.48
1:B:113:GLY:O	1:B:115:SER:N	2.47	0.48
1:C:351:VAL:HB	1:C:472:VAL:HG13	1.95	0.48
1:A:528:THR:HG22	1:A:530:VAL:N	2.22	0.48
1:A:187:VAL:HB	1:A:613:ALA:HB1	1.96	0.47
1:A:50:ASN:C	1:A:50:ASN:OD1	2.52	0.47
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.14	0.47
1:B:3:ARG:NH2	1:B:158:ASP:O	2.46	0.47
1:B:8:HIS:CE1	1:B:39:TYR:CE1	3.02	0.47
1:C:79:ALA:O	1:C:83:MET:HG2	2.14	0.47
1:D:176:LEU:HB2	1:D:177:PRO:HD3	1.96	0.47
1:C:589:ARG:NH1	1:C:589:ARG:CG	2.77	0.47
1:D:312:THR:HA	1:D:350:THR:O	2.14	0.47
1:A:484:ASN:ND2	1:A:484:ASN:N	2.63	0.47
1:B:360:LYS:HB3	1:B:448:VAL:HB	1.97	0.47
1:D:213:LEU:C	1:D:213:LEU:HD12	2.35	0.47
1:C:527:THR:OG1	1:C:528:THR:N	2.47	0.47
1:B:430:LEU:HD12	1:C:96:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:HD22	1:A:133:ASN:N	1.97	0.47
1:A:528:THR:CG2	1:A:530:VAL:H	2.23	0.47
1:B:484:ASN:ND2	1:B:484:ASN:N	2.58	0.47
1:D:291:GLU:HA	1:D:291:GLU:OE1	2.15	0.47
1:B:126:VAL:O	1:B:128:ILE:HG13	2.14	0.47
1:B:176:LEU:HB2	1:B:177:PRO:HD3	1.97	0.47
1:B:476:PHE:O	1:B:478:PRO:HD3	2.15	0.47
1:A:513:TYR:O	1:A:517:GLU:HG2	2.15	0.47
1:C:311:ASN:HD21	1:C:348:LYS:HD2	1.79	0.47
1:A:392:ARG:NH1	1:A:418:LYS:HD3	2.30	0.47
1:B:276:PHE:CD2	1:B:521:MET:HE3	2.50	0.47
1:A:349:LYS:O	1:A:471:ARG:HG3	2.15	0.47
1:C:10:LEU:HD23	1:C:43:TYR:CD1	2.50	0.47
1:A:183:ARG:HB2	1:A:183:ARG:HE	1.56	0.46
1:D:376:ARG:O	1:D:379:GLU:HB2	2.15	0.46
1:A:333:GLU:OE2	1:A:337:ARG:NH1	2.48	0.46
1:B:442:ILE:HD12	1:B:459:ILE:HG13	1.96	0.46
1:C:192:THR:HG22	1:C:246:THR:HG22	1.97	0.46
1:C:547:LYS:HB2	1:C:547:LYS:HE3	1.75	0.46
1:D:67:GLU:N	1:D:67:GLU:CD	2.69	0.46
1:D:575:PHE:O	1:D:578:LYS:HB2	2.15	0.46
1:D:549:TYR:C	1:D:590:THR:HG22	2.34	0.46
1:C:479:GLU:HG3	1:C:480:PHE:N	2.29	0.46
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.96	0.46
1:D:465:PHE:O	1:D:466:ASN:HB2	2.16	0.46
1:B:415:GLU:HG2	1:B:417:LEU:O	2.16	0.46
1:A:615:ARG:O	1:A:615:ARG:HD2	2.15	0.46
1:A:612:LEU:HD21	1:A:616:ARG:NH2	2.30	0.46
1:B:565:VAL:O	1:B:569:VAL:HG23	2.15	0.46
1:C:321:TYR:CD2	1:C:359:ALA:HB2	2.51	0.46
1:D:385:VAL:CG1	1:D:417:LEU:HD21	2.46	0.46
1:B:193:HIS:ND1	1:B:247:VAL:HG11	2.31	0.46
1:A:443:VAL:HG12	1:A:445:HIS:H	1.80	0.46
1:A:69:PHE:HD2	1:A:77:GLN:HE21	1.60	0.46
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.98	0.46
1:D:485:ASN:HA	1:D:486:PRO:HD3	1.84	0.46
1:A:119:LYS:HZ2	1:A:130:SER:HB2	1.81	0.45
1:A:386:THR:HG21	1:C:390:GLY:CA	2.46	0.45
1:A:484:ASN:ND2	1:A:484:ASN:H	2.14	0.45
1:B:334:ALA:CB	1:B:568:LEU:HD23	2.46	0.45
1:B:90:PHE:N	1:B:90:PHE:CD2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:HA	1:C:81:GLN:NE2	2.30	0.45
1:D:210:TYR:CZ	1:D:530:VAL:HB	2.51	0.45
1:D:443:VAL:HG22	1:D:456:LEU:HD21	1.97	0.45
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.98	0.45
1:D:576:VAL:C	1:D:578:LYS:H	2.19	0.45
1:B:514:THR:HB	1:B:515:PRO:HD3	1.98	0.45
1:C:479:GLU:HG3	1:C:480:PHE:H	1.81	0.45
1:D:17:VAL:HG23	1:D:18:ALA:N	2.32	0.45
1:D:40:LYS:HB3	1:D:41:ASP:H	1.52	0.45
1:A:210:TYR:CZ	1:A:530:VAL:HB	2.52	0.45
1:C:331:PHE:O	1:C:335:LEU:HB2	2.16	0.45
1:D:385:VAL:HG13	1:D:417:LEU:HD21	1.98	0.45
1:A:465:PHE:O	1:A:466:ASN:HB2	2.16	0.45
1:B:332:ILE:HG12	1:B:474:MET:HE1	1.97	0.45
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.99	0.45
1:D:134:ASP:CG	1:D:137:THR:HG23	2.37	0.45
1:D:3:ARG:NH1	1:D:185:ASP:OD2	2.49	0.45
1:A:213:LEU:HA	1:A:216:VAL:CG1	2.46	0.45
1:B:610:ARG:O	1:B:613:ALA:HB3	2.17	0.45
1:C:264:ASP:O	1:C:635:MET:HG3	2.17	0.45
1:C:3:ARG:NH2	1:C:158:ASP:O	2.49	0.45
1:C:559:LYS:HB3	1:C:563:GLU:HB2	1.99	0.45
1:D:385:VAL:CG2	1:D:421:ASP:HB3	2.47	0.45
1:A:330:MET:CE	1:A:568:LEU:HD22	2.46	0.45
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.51	0.45
1:B:74:ARG:N	1:B:75:PRO:CD	2.80	0.45
1:D:275:LYS:O	1:D:275:LYS:CG	2.63	0.45
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.47	0.45
1:B:181:LYS:C	1:B:183:ARG:H	2.20	0.45
1:B:8:HIS:CD2	1:B:614:LEU:HD11	2.52	0.45
1:C:21:VAL:CG1	1:C:21:VAL:O	2.64	0.45
1:C:471:ARG:HG3	1:C:471:ARG:HH11	1.81	0.45
1:D:311:ASN:HD21	1:D:348:LYS:HD2	1.81	0.45
1:B:266:ILE:CG2	1:B:268:PRO:HG3	2.47	0.45
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.50	0.45
1:B:397:ALA:HB1	1:D:429:ILE:HG12	1.98	0.45
1:A:150:PHE:O	1:A:154:VAL:HG23	2.17	0.45
1:D:250:ILE:HG12	1:D:530:VAL:HA	1.99	0.45
1:D:434:ARG:O	1:D:435:PRO:C	2.56	0.45
1:A:113:GLY:C	1:A:115:SER:H	2.21	0.44
1:A:208:ASP:OD2	1:A:209:PHE:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:TYR:HD2	1:C:359:ALA:HB2	1.81	0.44
1:C:593:LEU:O	1:C:594:SER:C	2.56	0.44
1:A:114:TYR:HD1	1:A:114:TYR:H	1.65	0.44
1:A:170:TRP:O	1:A:172:ALA:N	2.51	0.44
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.78	0.44
1:D:399:ARG:O	1:D:400:TYR:C	2.55	0.44
1:C:604:LEU:O	1:C:608:LYS:HG3	2.18	0.44
1:D:484:ASN:N	1:D:484:ASN:ND2	2.65	0.44
1:A:471:ARG:NE	1:A:471:ARG:HA	2.33	0.44
1:B:164:VAL:HA	1:B:187:VAL:HG23	1.99	0.44
1:B:537:MET:HG2	1:B:551:ILE:HD13	2.00	0.44
1:C:16:GLU:O	1:C:17:VAL:C	2.54	0.44
1:B:429:ILE:HG12	1:D:397:ALA:HB1	1.99	0.44
1:A:197:LEU:HA	1:A:197:LEU:HD23	1.63	0.44
1:B:193:HIS:O	1:B:194:ALA:HB2	2.18	0.44
1:B:227:ILE:CG2	1:B:227:ILE:O	2.65	0.44
1:A:587:ARG:O	1:A:591:GLU:HB2	2.18	0.44
1:C:213:LEU:HA	1:C:216:VAL:HG12	2.00	0.44
1:C:296:PHE:CE2	1:C:354:PHE:HE1	2.36	0.44
1:D:514:THR:HB	1:D:515:PRO:HD3	2.00	0.44
1:D:78:HIS:HA	1:D:81:GLN:HB2	2.00	0.44
1:C:31:LYS:NZ	1:C:35:THR:HG21	2.33	0.44
1:A:125:LEU:HD21	1:A:181:LYS:CB	2.47	0.44
1:B:385:VAL:HG13	1:B:417:LEU:HD21	1.98	0.44
1:B:528:THR:HG21	1:B:530:VAL:HG22	1.99	0.44
1:B:341:ARG:NH2	1:B:566:GLU:OE1	2.51	0.44
1:B:82:THR:O	1:B:85:SER:HB2	2.18	0.44
1:C:40:LYS:HB3	1:C:41:ASP:H	1.55	0.44
1:C:528:THR:CG2	1:C:530:VAL:H	2.22	0.44
1:C:81:GLN:CA	1:C:81:GLN:NE2	2.81	0.44
1:B:39:TYR:CB	1:B:43:TYR:HB2	2.48	0.43
1:B:11:PHE:CD1	1:B:46:ILE:HD11	2.53	0.43
1:C:289:LYS:HD2	1:C:289:LYS:N	2.31	0.43
1:C:78:HIS:HA	1:C:81:GLN:HB2	1.99	0.43
1:A:427:ARG:HD2	1:D:96:LEU:O	2.18	0.43
1:C:291:GLU:OE1	1:C:291:GLU:HA	2.19	0.43
1:D:74:ARG:N	1:D:75:PRO:CD	2.81	0.43
1:D:604:LEU:O	1:D:608:LYS:HG3	2.17	0.43
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.99	0.43
1:B:443:VAL:HG22	1:B:456:LEU:HD21	2.00	0.43
1:B:350:THR:HG1	1:B:471:ARG:HH12	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.48	0.43
1:B:99:GLY:O	1:B:100:ALA:C	2.56	0.43
1:C:335:LEU:HA	1:C:335:LEU:HD12	1.68	0.43
1:D:266:ILE:HG22	1:D:268:PRO:CD	2.48	0.43
1:D:296:PHE:CG	1:D:488:LEU:HD13	2.53	0.43
1:D:81:GLN:CA	1:D:81:GLN:NE2	2.81	0.43
1:A:3:ARG:NH2	1:A:155:ALA:O	2.52	0.43
1:B:167:PHE:N	1:B:167:PHE:CD2	2.87	0.43
1:B:266:ILE:HG22	1:B:268:PRO:HD3	2.01	0.43
1:B:440:PRO:HA	1:B:441:PRO:HD3	1.90	0.43
1:B:326:LYS:HE2	1:B:509:GLU:OE1	2.18	0.43
1:B:538:GLU:HB2	1:B:553:ILE:HD13	2.00	0.43
1:B:80:LEU:HB3	1:B:90:PHE:HZ	1.81	0.43
1:D:97:ILE:O	1:D:98:GLU:C	2.56	0.43
1:C:75:PRO:HG2	1:C:158:ASP:OD2	2.19	0.43
1:C:514:THR:N	1:C:515:PRO:CD	2.82	0.43
1:D:226:GLY:C	1:D:227:ILE:HD13	2.39	0.43
1:D:333:GLU:CG	1:D:337:ARG:NH1	2.82	0.43
1:A:265:GLY:O	1:A:266:ILE:HD13	2.19	0.43
1:C:348:LYS:HG3	1:C:348:LYS:H	1.57	0.43
1:C:36:VAL:O	1:C:36:VAL:HG12	2.18	0.43
1:C:74:ARG:N	1:C:75:PRO:CD	2.82	0.43
1:D:210:TYR:CE1	1:D:250:ILE:HD11	2.53	0.43
1:B:13:THR:HA	1:B:46:ILE:O	2.18	0.43
1:B:549:TYR:HE2	1:B:589:ARG:HD3	1.77	0.43
1:B:59:ASP:HB2	1:B:96:LEU:HD21	2.01	0.43
1:C:265:GLY:O	1:C:266:ILE:HD13	2.19	0.43
1:A:440:PRO:HA	1:A:441:PRO:HD3	1.93	0.43
1:B:456:LEU:HA	1:B:456:LEU:HD23	1.87	0.43
1:B:289:LYS:NZ	1:B:494:GLU:OE2	2.50	0.43
1:C:528:THR:O	1:C:534:GLY:HA3	2.19	0.43
1:A:114:TYR:N	1:A:114:TYR:CD1	2.87	0.42
1:B:20:ARG:HA	1:B:25:TYR:CD1	2.54	0.42
1:B:331:PHE:O	1:B:335:LEU:HB2	2.19	0.42
1:C:266:ILE:HG22	1:C:268:PRO:CD	2.48	0.42
1:C:34:ILE:HD12	1:C:34:ILE:HA	1.66	0.42
1:D:351:VAL:HB	1:D:472:VAL:HG13	2.01	0.42
1:B:266:ILE:O	1:B:268:PRO:HD3	2.19	0.42
1:D:293:ILE:O	1:D:297:VAL:HG23	2.20	0.42
1:A:299:GLY:HA2	1:A:375:VAL:CG2	2.37	0.42
1:B:40:LYS:HB3	1:B:41:ASP:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:HD11	1:D:610:ARG:HA	2.00	0.42
1:D:313:LEU:HA	1:D:500:HIS:CD2	2.54	0.42
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.85	0.42
1:A:589:ARG:NH1	1:A:589:ARG:CG	2.71	0.42
1:B:213:LEU:HD12	1:B:214:GLU:N	2.35	0.42
1:B:378:LEU:O	1:B:382:VAL:HG23	2.19	0.42
1:C:227:ILE:HG23	1:C:230:ARG:HB2	2.01	0.42
1:D:201:LEU:HD12	1:D:209:PHE:HE2	1.84	0.42
1:B:338:LEU:HG	1:B:338:LEU:O	2.20	0.42
1:B:515:PRO:O	1:B:518:CYS:HB3	2.19	0.42
1:B:615:ARG:HD3	1:B:622:PHE:CD1	2.54	0.42
1:C:133:ASN:N	1:C:133:ASN:ND2	2.62	0.42
1:A:164:VAL:HA	1:A:187:VAL:HG23	2.02	0.42
1:A:218:VAL:HG23	1:A:219:ASP:H	1.83	0.42
1:A:80:LEU:O	1:A:83:MET:HB2	2.18	0.42
1:B:81:GLN:O	1:B:85:SER:N	2.41	0.42
1:C:364:PHE:CE2	1:C:486:PRO:HD2	2.55	0.42
1:A:463:GLN:HG2	1:A:465:PHE:HE2	1.83	0.42
1:B:334:ALA:HB2	1:B:568:LEU:HD23	2.01	0.42
1:B:560:ALA:O	1:B:561:PRO:C	2.58	0.42
1:B:315:PHE:CE2	1:B:572:MET:HG2	2.55	0.42
1:C:321:TYR:C	1:C:321:TYR:CD1	2.93	0.42
1:D:561:PRO:O	1:D:564:SER:HB2	2.18	0.42
1:A:216:VAL:HG21	1:A:221:GLU:HG3	2.02	0.42
1:D:444:THR:OG1	1:D:445:HIS:CD2	2.69	0.42
1:A:275:LYS:O	1:A:275:LYS:CG	2.68	0.42
1:A:397:ALA:O	1:A:400:TYR:HB2	2.20	0.42
1:A:40:LYS:HB3	1:A:41:ASP:H	1.54	0.42
1:A:533:PHE:O	1:A:537:MET:HB2	2.19	0.42
1:B:368:ALA:HB1	1:B:487:ILE:CD1	2.49	0.42
1:A:455:ILE:O	1:A:459:ILE:HG12	2.20	0.42
1:B:5:LEU:N	1:B:5:LEU:HD23	2.34	0.42
1:C:181:LYS:HD3	1:C:181:LYS:O	2.20	0.42
1:A:127:GLY:O	1:A:129:PRO:HD3	2.20	0.41
1:C:321:TYR:C	1:C:321:TYR:HD1	2.23	0.41
1:D:552:TYR:HD1	1:D:571:TYR:CD2	2.39	0.41
1:A:181:LYS:O	1:A:183:ARG:N	2.53	0.41
1:A:459:ILE:H	1:A:459:ILE:HG12	1.71	0.41
1:A:551:ILE:HD12	1:A:593:LEU:HD13	2.02	0.41
1:B:332:ILE:HG23	1:B:459:ILE:HG22	2.01	0.41
1:C:301:PHE:HE1	1:C:473:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LEU:HD21	1:C:513:TYR:CE2	2.55	0.41
1:D:523:VAL:O	1:D:524:PRO:C	2.59	0.41
1:D:587:ARG:O	1:D:591:GLU:HB2	2.20	0.41
1:A:389:ILE:O	1:A:393:ILE:HG13	2.20	0.41
1:B:547:LYS:HB2	1:B:547:LYS:HE3	1.65	0.41
1:C:25:TYR:CD2	1:C:25:TYR:C	2.94	0.41
1:D:333:GLU:HG3	1:D:337:ARG:NH1	2.35	0.41
1:D:385:VAL:HG13	1:D:417:LEU:CD2	2.51	0.41
1:A:251:THR:O	1:A:254:GLU:HB2	2.21	0.41
1:A:429:ILE:HG12	1:C:397:ALA:HB1	2.02	0.41
1:B:266:ILE:HD13	1:B:266:ILE:HA	1.81	0.41
1:B:471:ARG:HH11	1:B:471:ARG:HG3	1.84	0.41
1:C:344:VAL:C	1:C:346:GLY:H	2.24	0.41
1:B:128:ILE:HA	1:B:129:PRO:HD3	1.75	0.41
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.86	0.41
1:B:612:LEU:HD11	1:B:616:ARG:HE	1.85	0.41
1:C:487:ILE:HG22	1:C:488:LEU:N	2.35	0.41
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.02	0.41
1:D:321:TYR:CD1	1:D:321:TYR:C	2.94	0.41
1:D:330:MET:CE	1:D:568:LEU:HD22	2.51	0.41
1:A:312:THR:HA	1:A:350:THR:O	2.21	0.41
1:A:514:THR:HB	1:A:515:PRO:HD3	2.03	0.41
1:A:493:ASP:CB	1:A:521:MET:CE	2.97	0.41
1:A:74:ARG:N	1:A:75:PRO:CD	2.84	0.41
1:C:6:GLN:HE21	1:C:6:GLN:HB2	1.66	0.41
1:A:274:ILE:H	1:A:274:ILE:HG13	1.62	0.41
1:A:474:MET:C	1:A:475:ILE:HG12	2.40	0.41
1:B:125:LEU:O	1:B:126:VAL:HG22	2.19	0.41
1:C:213:LEU:HD12	1:C:214:GLU:N	2.36	0.41
1:C:62:ASP:HB3	1:C:65:LYS:HG3	2.02	0.41
1:D:320:ARG:O	1:D:322:GLU:N	2.52	0.41
1:D:528:THR:CG2	1:D:530:VAL:HG22	2.51	0.41
1:A:364:PHE:CD1	1:A:487:ILE:HD12	2.56	0.41
1:C:372:GLN:O	1:C:376:ARG:HB2	2.21	0.41
1:D:434:ARG:HA	1:D:434:ARG:HD2	1.61	0.41
1:D:49:LEU:HD12	1:D:49:LEU:HA	1.87	0.41
1:D:74:ARG:NH2	1:D:77:GLN:HE22	2.08	0.41
1:A:41:ASP:OD1	1:A:102:LYS:HD2	2.21	0.41
1:B:3:ARG:HH12	1:B:185:ASP:HB3	1.86	0.41
1:C:554:VAL:CG1	1:C:555:ASP:N	2.84	0.41
1:C:565:VAL:O	1:C:569:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:GLN:HB3	1:C:621:GLN:HE21	1.68	0.41
1:D:218:VAL:HG23	1:D:219:ASP:H	1.85	0.41
1:D:323:TYR:OH	1:D:458:LYS:HG3	2.21	0.41
1:D:364:PHE:CD1	1:D:487:ILE:HD12	2.55	0.41
1:D:34:ILE:HD12	1:D:34:ILE:HA	1.67	0.40
1:D:3:ARG:NH1	1:D:185:ASP:CG	2.75	0.40
1:A:418:LYS:HG2	1:A:418:LYS:H	1.76	0.40
1:A:81:GLN:HA	1:A:81:GLN:NE2	2.27	0.40
1:B:19:ASN:N	1:B:19:ASN:HD22	2.19	0.40
1:C:14:ALA:HB2	1:C:168:HIS:HB2	2.02	0.40
1:C:316:PHE:CZ	1:C:496:VAL:HG22	2.56	0.40
1:D:213:LEU:HA	1:D:216:VAL:HG12	2.02	0.40
1:A:312:THR:HG22	1:A:350:THR:CB	2.36	0.40
1:B:286:HIS:O	1:B:287:ALA:C	2.59	0.40
1:C:309:LEU:HA	1:C:309:LEU:HD23	1.93	0.40
1:C:332:ILE:HG23	1:C:459:ILE:HG22	2.04	0.40
1:C:549:TYR:HA	1:C:549:TYR:HD2	1.67	0.40
1:D:16:GLU:O	1:D:17:VAL:C	2.59	0.40
1:D:8:HIS:CE1	1:D:39:TYR:HE1	2.40	0.40
1:B:234:GLU:HG2	1:B:259:LEU:HD21	2.03	0.40
1:D:274:ILE:HG13	1:D:274:ILE:H	1.68	0.40
1:D:300:HIS:HE1	1:D:441:PRO:O	2.04	0.40
1:D:537:MET:HG2	1:D:551:ILE:HD13	2.04	0.40
1:D:6:GLN:HE21	1:D:6:GLN:HB2	1.68	0.40
1:D:74:ARG:O	1:D:75:PRO:C	2.57	0.40
1:A:444:THR:OG1	1:A:445:HIS:CD2	2.70	0.40
1:A:321:TYR:CZ	1:A:455:ILE:HG13	2.57	0.40
1:A:550:GLY:HA3	1:A:590:THR:HG21	2.02	0.40
1:B:259:LEU:O	1:B:260:LYS:CB	2.69	0.40
1:C:267:LEU:HD21	1:C:606:TYR:HA	2.03	0.40
1:D:327:GLY:HA3	1:D:505:PRO:O	2.20	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	601/725 (83%)	541 (90%)	51 (8%)	9 (2%)	10	32
1	B	602/725 (83%)	543 (90%)	55 (9%)	4 (1%)	22	52
1	C	603/725 (83%)	549 (91%)	49 (8%)	5 (1%)	19	48
1	D	602/725 (83%)	547 (91%)	46 (8%)	9 (2%)	10	32
All	All	2408/2900 (83%)	2180 (90%)	201 (8%)	27 (1%)	14	40

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	SER
1	B	114	TYR
1	D	275	LYS
1	A	171	LEU
1	A	182	ARG
1	A	577	LYS
1	C	17	VAL
1	C	323	TYR
1	D	17	VAL
1	D	577	LYS
1	A	114	TYR
1	B	194	ALA
1	C	321	TYR
1	C	363	SER
1	D	415	GLU
1	A	194	ALA
1	C	594	SER
1	D	194	ALA
1	D	363	SER
1	A	435	PRO
1	D	490	LEU
1	A	274	ILE
1	B	126	VAL
1	B	363	SER
1	D	274	ILE
1	D	435	PRO
1	A	126	VAL

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%)	470 (89%)	56 (11%)	6	19
1	B	526/622 (85%)	467 (89%)	59 (11%)	6	16
1	C	527/622 (85%)	469 (89%)	58 (11%)	6	17
1	D	526/622 (85%)	474 (90%)	52 (10%)	8	22
All	All	2105/2488 (85%)	1880 (89%)	225 (11%)	6	18

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	ASN
1	A	19	ASN
1	A	35	THR
1	A	45	LEU
1	A	60	ILE
1	A	81	GLN
1	A	84	GLU
1	A	86	ARG
1	A	94	ARG
1	A	114	TYR
1	A	122	LEU
1	A	124	SER
1	A	125	LEU
1	A	133	ASN
1	A	136	GLU
1	A	183	ARG
1	A	216	VAL
1	A	247	VAL
1	A	272	ASN
1	A	277	GLN
1	A	289	LYS
1	A	291	GLU
1	A	304	CYS

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Mol	Chain	Res	Type
1	A	312	THR
1	A	321	TYR
1	A	335	LEU
1	A	348	LYS
1	A	363	SER
1	A	366	VAL
1	A	376	ARG
1	A	388	SER
1	A	395	ASP
1	A	399	ARG
1	A	400	TYR
1	A	418	LYS
1	A	434	ARG
1	A	436	GLU
1	A	458	LYS
1	A	459	ILE
1	A	469	SER
1	A	471	ARG
1	A	484	ASN
1	A	488	LEU
1	A	513	TYR
1	A	514	THR
1	A	525	SER
1	A	531	SER
1	A	533	PHE
1	A	562	ASP
1	A	564	SER
1	A	589	ARG
1	A	590	THR
1	A	621	GLN
1	A	629	GLU
1	A	633	SER
1	B	3	ARG
1	B	7	ASN
1	B	19	ASN
1	B	35	THR
1	B	40	LYS
1	B	42	HIS
1	B	60	ILE
1	B	72	GLU
1	B	74	ARG
1	B	85	SER

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Mol	Chain	Res	Type
1	B	86	ARG
1	B	111	VAL
1	B	114	TYR
1	B	122	LEU
1	B	125	LEU
1	B	133	ASN
1	B	183	ARG
1	B	199	ARG
1	B	216	VAL
1	B	272	ASN
1	B	289	LYS
1	B	291	GLU
1	B	312	THR
1	B	320	ARG
1	B	321	TYR
1	B	326	LYS
1	B	348	LYS
1	B	366	VAL
1	B	376	ARG
1	B	387	THR
1	B	388	SER
1	B	395	ASP
1	B	399	ARG
1	B	400	TYR
1	B	418	LYS
1	B	423	VAL
1	B	426	LYS
1	B	434	ARG
1	B	436	GLU
1	B	443	VAL
1	B	448	VAL
1	B	458	LYS
1	B	459	ILE
1	B	469	SER
1	B	471	ARG
1	B	472	VAL
1	B	484	ASN
1	B	488	LEU
1	B	493	ASP
1	B	513	TYR
1	B	525	SER
1	B	548	ASP

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Mol	Chain	Res	Type
1	B	556	ARG
1	B	564	SER
1	B	574	GLU
1	B	590	THR
1	B	621	GLN
1	B	629	GLU
1	B	633	SER
1	C	6	GLN
1	C	7	ASN
1	C	19	ASN
1	C	34	ILE
1	C	40	LYS
1	C	42	HIS
1	C	60	ILE
1	C	72	GLU
1	C	74	ARG
1	C	81	GLN
1	C	84	GLU
1	C	111	VAL
1	C	122	LEU
1	C	133	ASN
1	C	136	GLU
1	C	183	ARG
1	C	199	ARG
1	C	213	LEU
1	C	216	VAL
1	C	289	LYS
1	C	291	GLU
1	C	320	ARG
1	C	321	TYR
1	C	326	LYS
1	C	335	LEU
1	C	343	LYS
1	C	348	LYS
1	C	363	SER
1	C	376	ARG
1	C	395	ASP
1	C	399	ARG
1	C	400	TYR
1	C	418	LYS
1	C	419	SER
1	C	426	LYS

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Mol	Chain	Res	Type
1	C	436	GLU
1	C	443	VAL
1	C	458	LYS
1	C	459	ILE
1	C	461	GLN
1	C	469	SER
1	C	471	ARG
1	C	472	VAL
1	C	482	ASN
1	C	488	LEU
1	C	490	LEU
1	C	513	TYR
1	C	514	THR
1	C	525	SER
1	C	537	MET
1	C	549	TYR
1	C	556	ARG
1	C	562	ASP
1	C	578	LYS
1	C	587	ARG
1	C	590	THR
1	C	633	SER
1	C	635	MET
1	D	7	ASN
1	D	15	THR
1	D	19	ASN
1	D	34	ILE
1	D	42	HIS
1	D	60	ILE
1	D	81	GLN
1	D	84	GLU
1	D	85	SER
1	D	111	VAL
1	D	122	LEU
1	D	124	SER
1	D	133	ASN
1	D	137	THR
1	D	183	ARG
1	D	216	VAL
1	D	289	LYS
1	D	291	GLU
1	D	304	CYS

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Mol	Chain	Res	Type
1	D	320	ARG
1	D	321	TYR
1	D	326	LYS
1	D	335	LEU
1	D	348	LYS
1	D	363	SER
1	D	376	ARG
1	D	395	ASP
1	D	399	ARG
1	D	400	TYR
1	D	426	LYS
1	D	434	ARG
1	D	436	GLU
1	D	458	LYS
1	D	459	ILE
1	D	471	ARG
1	D	472	VAL
1	D	482	ASN
1	D	484	ASN
1	D	513	TYR
1	D	514	THR
1	D	525	SER
1	D	528	THR
1	D	537	MET
1	D	556	ARG
1	D	562	ASP
1	D	563	GLU
1	D	587	ARG
1	D	590	THR
1	D	621	GLN
1	D	629	GLU
1	D	632	ASP
1	D	633	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	HIS
1	A	81	GLN
1	A	133	ASN
1	A	239	HIS

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Mol	Chain	Res	Type
1	A	249	GLN
1	A	300	HIS
1	A	311	ASN
1	A	445	HIS
1	A	484	ASN
1	A	500	HIS
1	A	621	GLN
1	B	6	GLN
1	B	8	HIS
1	B	77	GLN
1	B	133	ASN
1	B	300	HIS
1	B	445	HIS
1	B	482	ASN
1	B	484	ASN
1	B	500	HIS
1	B	621	GLN
1	C	6	GLN
1	C	8	HIS
1	C	77	GLN
1	C	81	GLN
1	C	133	ASN
1	C	239	HIS
1	C	249	GLN
1	C	257	HIS
1	C	300	HIS
1	C	311	ASN
1	C	445	HIS
1	C	484	ASN
1	C	500	HIS
1	C	621	GLN
1	D	6	GLN
1	D	8	HIS
1	D	19	ASN
1	D	77	GLN
1	D	81	GLN
1	D	89	HIS
1	D	133	ASN
1	D	239	HIS
1	D	249	GLN
1	D	300	HIS
1	D	311	ASN

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Mol	Chain	Res	Type
1	D	445	HIS
1	D	477	HIS
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	D	804	-	4,4,4	0.14	0	6,6,6	0.18	0
2	SO4	A	804	-	4,4,4	0.19	0	6,6,6	0.14	0
2	SO4	A	803	-	4,4,4	0.28	0	6,6,6	0.41	0
2	SO4	C	804	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	B	803	-	4,4,4	0.30	0	6,6,6	0.49	0
2	SO4	A	801	-	4,4,4	0.30	0	6,6,6	0.43	0
2	SO4	D	803	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	C	802	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	D	802	-	4,4,4	0.27	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	802	-	4,4,4	0.28	0	6,6,6	0.29	0
2	SO4	B	802	-	4,4,4	0.14	0	6,6,6	0.42	0
2	SO4	C	801	-	4,4,4	0.22	0	6,6,6	0.37	0
2	SO4	B	801	-	4,4,4	0.29	0	6,6,6	0.20	0
2	SO4	C	803	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	D	801	-	4,4,4	0.31	0	6,6,6	0.56	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	802	SO4	1	0
2	A	802	SO4	1	0
2	B	802	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	611/725 (84%)	0.19	19 (3%)	49 45	48, 69, 93, 123	0
1	B	612/725 (84%)	0.21	22 (3%)	42 38	53, 71, 93, 122	0
1	C	613/725 (84%)	0.09	20 (3%)	46 41	49, 68, 93, 120	0
1	D	612/725 (84%)	0.10	10 (1%)	72 71	44, 66, 93, 122	0
All	All	2448/2900 (84%)	0.15	71 (2%)	51 48	44, 69, 93, 123	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	630	LEU	5.0
1	B	416	LEU	5.0
1	B	630	LEU	4.7
1	D	416	LEU	4.7
1	C	414	GLY	4.7
1	A	630	LEU	4.0
1	D	630	LEU	4.0
1	C	415	GLU	3.8
1	A	416	LEU	3.7
1	C	417	LEU	3.7
1	D	625	LEU	3.7
1	A	549	TYR	3.7
1	B	627	GLY	3.6
1	B	414	GLY	3.6
1	B	581	ALA	3.6
1	B	549	TYR	3.5
1	A	624	GLU	3.3
1	C	624	GLU	3.3
1	C	416	LEU	3.2
1	B	135	PHE	3.2
1	A	627	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	625	LEU	3.1
1	A	629	GLU	3.1
1	C	629	GLU	3.1
1	C	549	TYR	3.1
1	B	628	GLU	3.0
1	D	627	GLY	3.0
1	D	549	TYR	2.9
1	C	638	LEU	2.9
1	C	626	VAL	2.9
1	B	580	ALA	2.9
1	B	631	ASN	2.9
1	B	626	VAL	2.9
1	A	628	GLU	2.8
1	C	313	LEU	2.8
1	C	436	GLU	2.7
1	A	548	ASP	2.7
1	A	631	ASN	2.6
1	B	624	GLU	2.6
1	A	417	LEU	2.6
1	B	623	ARG	2.6
1	A	132	GLU	2.6
1	B	622	PHE	2.6
1	A	344	VAL	2.5
1	C	628	GLU	2.5
1	D	626	VAL	2.5
1	B	629	GLU	2.5
1	C	581	ALA	2.5
1	D	313	LEU	2.5
1	B	305	PHE	2.4
1	C	631	ASN	2.4
1	D	624	GLU	2.3
1	A	135	PHE	2.3
1	B	225	PHE	2.3
1	D	415	GLU	2.3
1	B	342	LEU	2.3
1	C	625	LEU	2.3
1	C	637	ALA	2.3
1	A	626	VAL	2.2
1	C	627	GLY	2.2
1	C	6	GLN	2.2
1	A	340	TYR	2.2
1	D	628	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	6	GLN	2.1
1	C	639	ALA	2.1
1	B	132	GLU	2.1
1	A	225	PHE	2.1
1	B	133	ASN	2.1
1	B	131	PRO	2.1
1	B	344	VAL	2.0
1	A	540	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	D	801	5/5	0.75	0.30	82,84,92,103	0
2	SO4	C	804	5/5	0.82	0.28	103,109,110,117	0
2	SO4	D	804	5/5	0.86	0.27	105,108,116,121	0
2	SO4	B	803	5/5	0.87	0.17	77,86,88,97	0
2	SO4	C	801	5/5	0.89	0.20	85,86,90,103	0
2	SO4	A	803	5/5	0.90	0.18	76,80,85,91	0
2	SO4	A	801	5/5	0.90	0.24	71,76,84,92	0
2	SO4	C	803	5/5	0.91	0.19	90,91,97,105	0
2	SO4	A	804	5/5	0.92	0.17	100,101,104,108	0
2	SO4	D	803	5/5	0.92	0.18	82,88,94,100	0
2	SO4	D	802	5/5	0.92	0.14	77,79,87,92	0
2	SO4	B	801	5/5	0.95	0.16	72,77,83,91	0
2	SO4	C	802	5/5	0.96	0.15	76,77,90,91	0
2	SO4	A	802	5/5	0.96	0.18	68,71,75,77	0
2	SO4	B	802	5/5	0.97	0.12	71,75,81,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.