Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 11:51 PM EDT

PDB ID	:	3LCW
Title	:	L-KDO aldolase complexed with hydroxypyruvate
Authors	:	Chou, C.-Y.; Wang, A.H.-J.; Ko, T.-P.
Deposited on	:	2010-01-12
Resolution	:	2.35 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

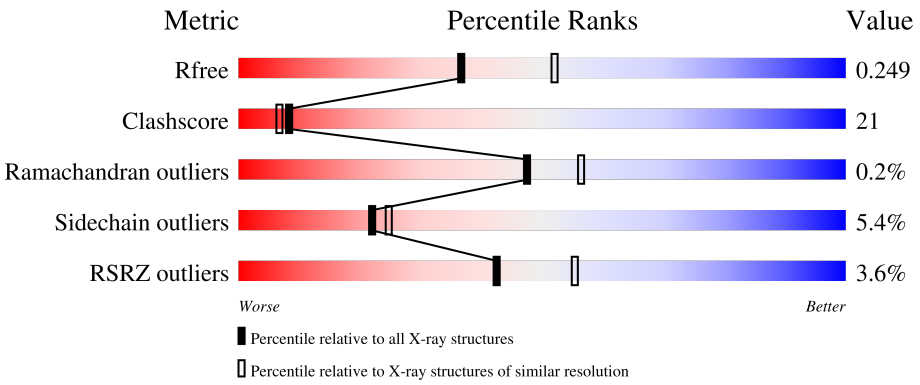
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	319	% 59% 30% • 9%
1	B	319	5% 62% 26% • 9%
1	C	319	7% 57% 32% • 9%
1	D	319	% 56% 32% • 9%

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	3PY	B	641	-	X	-	-
2	3PY	C	642	-	X	-	-
2	3PY	D	643	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9473 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 N-acetylneuraminate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	291	2234	1425	380	418	11	71	0	0
1	B	291	2234	1425	380	418	11	70	0	0
1	C	291	2234	1425	380	418	11	68	0	0
1	D	291	2234	1425	380	418	11	54	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P0A6L4
A	-20	GLY	-	expression tag	UNP P0A6L4
A	-19	HIS	-	expression tag	UNP P0A6L4
A	-18	HIS	-	expression tag	UNP P0A6L4
A	-17	HIS	-	expression tag	UNP P0A6L4
A	-16	HIS	-	expression tag	UNP P0A6L4
A	-15	HIS	-	expression tag	UNP P0A6L4
A	-14	HIS	-	expression tag	UNP P0A6L4
A	-13	HIS	-	expression tag	UNP P0A6L4
A	-12	HIS	-	expression tag	UNP P0A6L4
A	-11	HIS	-	expression tag	UNP P0A6L4
A	-10	HIS	-	expression tag	UNP P0A6L4
A	-9	SER	-	expression tag	UNP P0A6L4
A	-8	SER	-	expression tag	UNP P0A6L4
A	-7	GLY	-	expression tag	UNP P0A6L4
A	-6	HIS	-	expression tag	UNP P0A6L4
A	-5	ILE	-	expression tag	UNP P0A6L4
A	-4	GLU	-	expression tag	UNP P0A6L4
A	-3	GLY	-	expression tag	UNP P0A6L4
A	-2	ARG	-	expression tag	UNP P0A6L4
A	-1	HIS	-	expression tag	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P0A6L4
A	60	ALA	GLU	engineered mutation	UNP P0A6L4
A	98	HIS	TYR	engineered mutation	UNP P0A6L4
A	115	LEU	PHE	engineered mutation	UNP P0A6L4
A	150	GLY	ASP	engineered mutation	UNP P0A6L4
A	153	TYR	ASN	engineered mutation	UNP P0A6L4
A	251	ILE	VAL	engineered mutation	UNP P0A6L4
A	265	ILE	VAL	engineered mutation	UNP P0A6L4
A	281	CYS	TYR	engineered mutation	UNP P0A6L4
B	-21	MET	-	expression tag	UNP P0A6L4
B	-20	GLY	-	expression tag	UNP P0A6L4
B	-19	HIS	-	expression tag	UNP P0A6L4
B	-18	HIS	-	expression tag	UNP P0A6L4
B	-17	HIS	-	expression tag	UNP P0A6L4
B	-16	HIS	-	expression tag	UNP P0A6L4
B	-15	HIS	-	expression tag	UNP P0A6L4
B	-14	HIS	-	expression tag	UNP P0A6L4
B	-13	HIS	-	expression tag	UNP P0A6L4
B	-12	HIS	-	expression tag	UNP P0A6L4
B	-11	HIS	-	expression tag	UNP P0A6L4
B	-10	HIS	-	expression tag	UNP P0A6L4
B	-9	SER	-	expression tag	UNP P0A6L4
B	-8	SER	-	expression tag	UNP P0A6L4
B	-7	GLY	-	expression tag	UNP P0A6L4
B	-6	HIS	-	expression tag	UNP P0A6L4
B	-5	ILE	-	expression tag	UNP P0A6L4
B	-4	GLU	-	expression tag	UNP P0A6L4
B	-3	GLY	-	expression tag	UNP P0A6L4
B	-2	ARG	-	expression tag	UNP P0A6L4
B	-1	HIS	-	expression tag	UNP P0A6L4
B	0	MET	-	expression tag	UNP P0A6L4
B	60	ALA	GLU	engineered mutation	UNP P0A6L4
B	98	HIS	TYR	engineered mutation	UNP P0A6L4
B	115	LEU	PHE	engineered mutation	UNP P0A6L4
B	150	GLY	ASP	engineered mutation	UNP P0A6L4
B	153	TYR	ASN	engineered mutation	UNP P0A6L4
B	251	ILE	VAL	engineered mutation	UNP P0A6L4
B	265	ILE	VAL	engineered mutation	UNP P0A6L4
B	281	CYS	TYR	engineered mutation	UNP P0A6L4
C	-21	MET	-	expression tag	UNP P0A6L4
C	-20	GLY	-	expression tag	UNP P0A6L4
C	-19	HIS	-	expression tag	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP P0A6L4
C	-17	HIS	-	expression tag	UNP P0A6L4
C	-16	HIS	-	expression tag	UNP P0A6L4
C	-15	HIS	-	expression tag	UNP P0A6L4
C	-14	HIS	-	expression tag	UNP P0A6L4
C	-13	HIS	-	expression tag	UNP P0A6L4
C	-12	HIS	-	expression tag	UNP P0A6L4
C	-11	HIS	-	expression tag	UNP P0A6L4
C	-10	HIS	-	expression tag	UNP P0A6L4
C	-9	SER	-	expression tag	UNP P0A6L4
C	-8	SER	-	expression tag	UNP P0A6L4
C	-7	GLY	-	expression tag	UNP P0A6L4
C	-6	HIS	-	expression tag	UNP P0A6L4
C	-5	ILE	-	expression tag	UNP P0A6L4
C	-4	GLU	-	expression tag	UNP P0A6L4
C	-3	GLY	-	expression tag	UNP P0A6L4
C	-2	ARG	-	expression tag	UNP P0A6L4
C	-1	HIS	-	expression tag	UNP P0A6L4
C	0	MET	-	expression tag	UNP P0A6L4
C	60	ALA	GLU	engineered mutation	UNP P0A6L4
C	98	HIS	TYR	engineered mutation	UNP P0A6L4
C	115	LEU	PHE	engineered mutation	UNP P0A6L4
C	150	GLY	ASP	engineered mutation	UNP P0A6L4
C	153	TYR	ASN	engineered mutation	UNP P0A6L4
C	251	ILE	VAL	engineered mutation	UNP P0A6L4
C	265	ILE	VAL	engineered mutation	UNP P0A6L4
C	281	CYS	TYR	engineered mutation	UNP P0A6L4
D	-21	MET	-	expression tag	UNP P0A6L4
D	-20	GLY	-	expression tag	UNP P0A6L4
D	-19	HIS	-	expression tag	UNP P0A6L4
D	-18	HIS	-	expression tag	UNP P0A6L4
D	-17	HIS	-	expression tag	UNP P0A6L4
D	-16	HIS	-	expression tag	UNP P0A6L4
D	-15	HIS	-	expression tag	UNP P0A6L4
D	-14	HIS	-	expression tag	UNP P0A6L4
D	-13	HIS	-	expression tag	UNP P0A6L4
D	-12	HIS	-	expression tag	UNP P0A6L4
D	-11	HIS	-	expression tag	UNP P0A6L4
D	-10	HIS	-	expression tag	UNP P0A6L4
D	-9	SER	-	expression tag	UNP P0A6L4
D	-8	SER	-	expression tag	UNP P0A6L4
D	-7	GLY	-	expression tag	UNP P0A6L4

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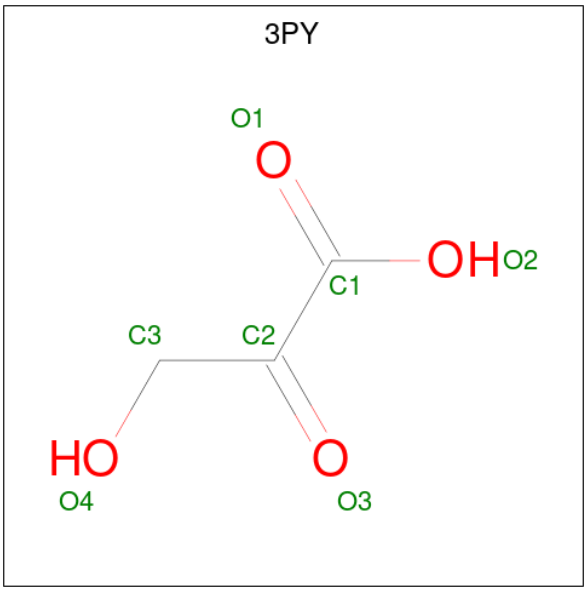
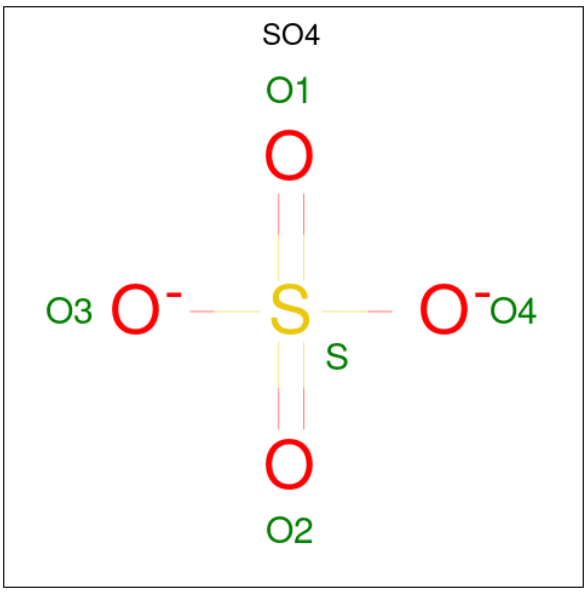
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP P0A6L4
D	-5	ILE	-	expression tag	UNP P0A6L4
D	-4	GLU	-	expression tag	UNP P0A6L4
D	-3	GLY	-	expression tag	UNP P0A6L4
D	-2	ARG	-	expression tag	UNP P0A6L4
D	-1	HIS	-	expression tag	UNP P0A6L4
D	0	MET	-	expression tag	UNP P0A6L4
D	60	ALA	GLU	engineered mutation	UNP P0A6L4
D	98	HIS	TYR	engineered mutation	UNP P0A6L4
D	115	LEU	PHE	engineered mutation	UNP P0A6L4
D	150	GLY	ASP	engineered mutation	UNP P0A6L4
D	153	TYR	ASN	engineered mutation	UNP P0A6L4
D	251	ILE	VAL	engineered mutation	UNP P0A6L4
D	265	ILE	VAL	engineered mutation	UNP P0A6L4
D	281	CYS	TYR	engineered mutation	UNP P0A6L4

- Molecule 2 is 3-HYDROXYPYRUVIC ACID (three-letter code: 3PY) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	B	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

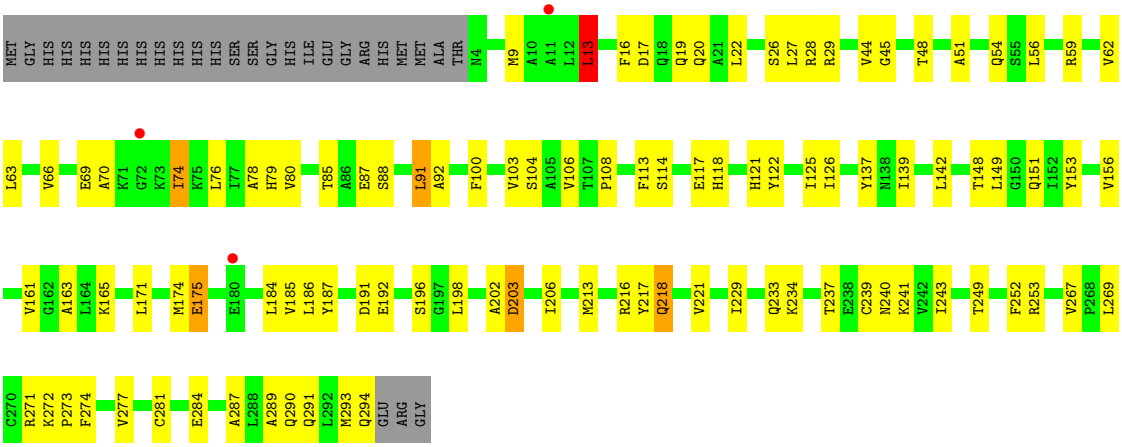
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	146	146	146	0	0
4	B	113	113	113	0	0
4	C	108	108	108	0	0
4	D	126	126	126	0	0

3 Residue-property plots (i)

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

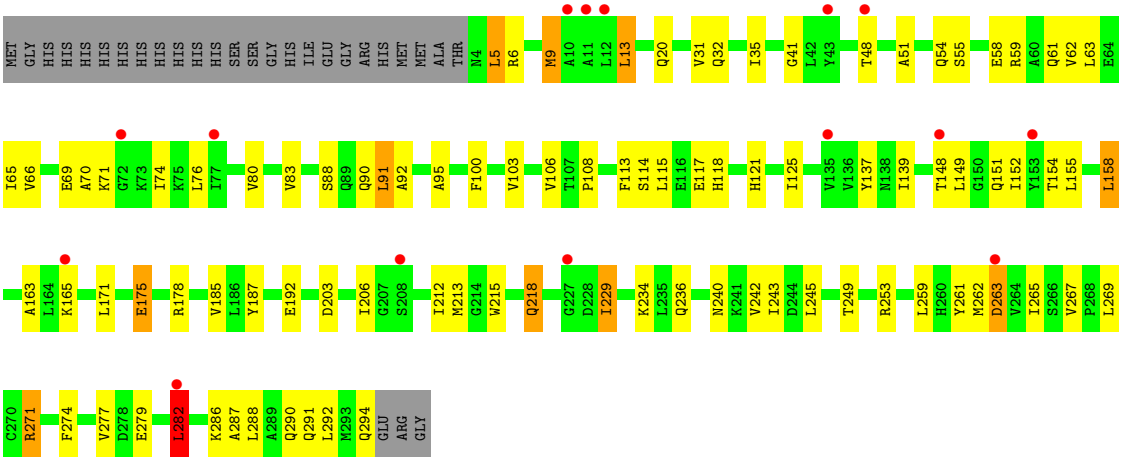
• Molecule 1: N-acetylneuraminate lyase

Chain A:



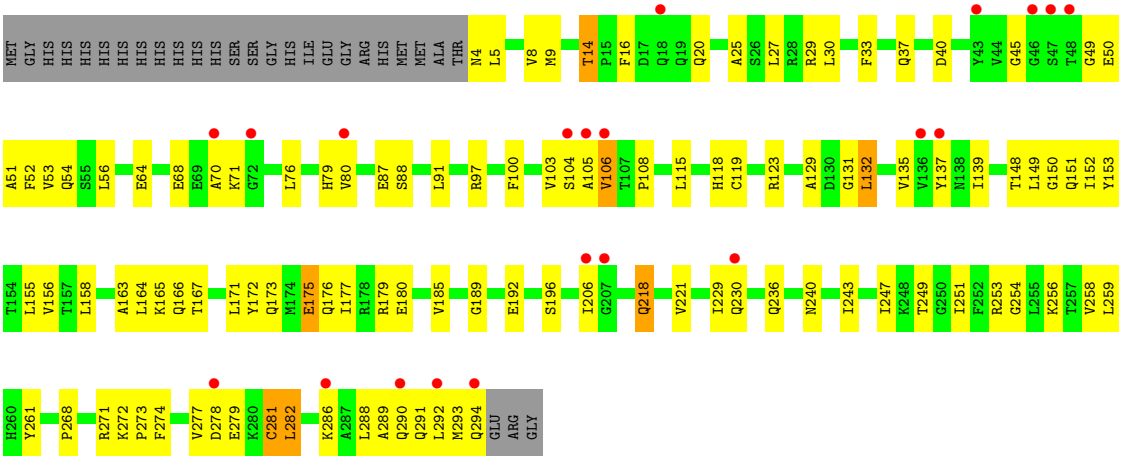
• Molecule 1: N-acetylneuraminate lyase

Chain B:



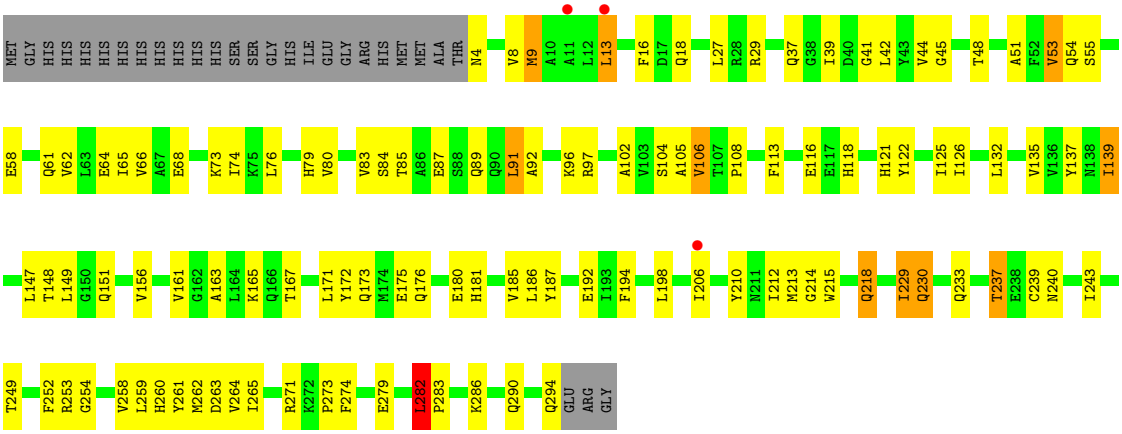
• Molecule 1: N-acetylneuraminate lyase

Chain C:



- Molecule 1: N-acetylneuraminate lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.83Å 120.83Å 195.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.83 – 2.35 27.83 – 2.35	Depositor EDS
% Data completeness (in resolution range)	90.6 (27.83-2.35) 95.4 (27.83-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.41 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.274 0.210 , 0.249	Depositor DCC
R_{free} test set	3366 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9473	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 3PY, 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	0.37	0/2273	0.63	1/3076 (0.0%)
1	B	0.37	1/2273 (0.0%)	0.62	1/3076 (0.0%)
1	C	0.35	0/2273	0.63	1/3076 (0.0%)
1	D	0.40	1/2273 (0.0%)	0.64	1/3076 (0.0%)
All	All	0.37	2/9092 (0.0%)	0.63	4/12304 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	282	LEU	C-N	8.08	1.49	1.34
1	B	282	LEU	C-N	7.05	1.47	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	LEU	CA-CB-CG	6.67	130.63	115.30
1	D	13	LEU	CA-CB-CG	6.43	130.09	115.30
1	B	13	LEU	CA-CB-CG	5.62	128.24	115.30
1	C	281	CYS	O-C-N	-5.14	114.48	122.70

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	2234	0	2268	103	0
1	B	2234	0	2268	77	0
1	C	2234	0	2268	100	0
1	D	2234	0	2268	102	0
2	A	6	0	2	0	0
2	B	6	0	2	0	0
2	C	6	0	2	0	0
2	D	6	0	2	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
4	A	146	0	0	3	0
4	B	113	0	0	1	0
4	C	108	0	0	3	0
4	D	126	0	0	9	0
All	All	9473	0	9080	365	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 21.

All (365) 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:C:80:VAL:HG13	1:C:91:LEU:HB3	1.29	1.10
1:A:218:GLN:HE21	1:A:218:GLN:HA	1.29	0.95
1:A:20:GLN:HE22	1:A:272:LYS:H	1.05	0.94
1:A:80:VAL:HG13	1:A:91:LEU:HB3	1.51	0.91
1:D:192:GLU:HG3	1:D:243:ILE:HD13	1.56	0.87
1:C:218:GLN:HE21	1:C:218:GLN:HA	1.38	0.86
1:A:213:MET:HE1	1:A:216:ARG:HH11	1.41	0.86
1:B:80:VAL:HG13	1:B:91:LEU:CB	2.08	0.83
1:B:115:LEU:HD11	1:B:154:THR:HG21	1.61	0.82
1:A:213:MET:HE3	1:A:216:ARG:HD2	1.63	0.81
1:B:218:GLN:HE21	1:B:218:GLN:HA	1.45	0.80
1:C:80:VAL:HG13	1:C:91:LEU:CB	2.12	0.80
1:C:79:HIS:HE1	1:C:106:VAL:H	1.31	0.79
1:C:56:LEU:HD11	1:C:87:GLU:HG2	1.64	0.79
1:D:106:VAL:HG13	1:D:137:TYR:CD2	2.17	0.79
1:B:80:VAL:HG13	1:B:91:LEU:HB3	1.65	0.78
1:D:108:PRO:HD2	1:D:118:HIS:HD2	1.47	0.78
1:D:258:VAL:O	1:D:262:MET:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:HD2	1:A:118:HIS:HD2	1.51	0.75
1:C:106:VAL:HG13	1:C:137:TYR:CD2	2.20	0.75
1:A:70:ALA:HB1	1:A:74:ILE:CD1	2.16	0.75
1:C:279:GLU:HA	1:C:282:LEU:HD23	1.67	0.74
1:D:249:THR:O	1:D:253:ARG:HD2	1.88	0.74
1:A:121:HIS:O	1:A:125:ILE:HG12	1.87	0.74
1:D:79:HIS:HE1	1:D:106:VAL:H	1.36	0.74
1:A:20:GLN:NE2	1:A:272:LYS:H	1.84	0.74
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.53	0.73
1:A:249:THR:O	1:A:253:ARG:HD2	1.89	0.72
1:C:218:GLN:HA	1:C:218:GLN:NE2	2.04	0.72
1:A:80:VAL:HG13	1:A:91:LEU:CB	2.20	0.71
1:A:108:PRO:HD2	1:A:118:HIS:CD2	2.25	0.71
1:D:192:GLU:HA	1:D:240:ASN:HD21	1.55	0.71
1:C:271:ARG:O	1:C:274:PHE:HB2	1.91	0.70
1:D:279:GLU:HA	1:D:282:LEU:CD2	2.20	0.70
1:C:261:TYR:CZ	1:C:286:LYS:HG2	2.28	0.69
1:C:79:HIS:CE1	1:C:106:VAL:HG22	2.27	0.69
1:A:79:HIS:HE1	1:A:106:VAL:H	1.41	0.69
1:D:233:GLN:O	1:D:237:THR:HG23	1.93	0.69
1:D:79:HIS:CE1	1:D:106:VAL:HG22	2.27	0.68
1:D:264:VAL:HG12	1:D:265:ILE:HD12	1.76	0.68
1:A:186:LEU:H	1:A:203:ASP:HB2	1.58	0.68
1:B:62:VAL:O	1:B:66:VAL:HG12	1.94	0.68
1:C:129:ALA:O	1:C:132:LEU:HD13	1.94	0.67
1:A:114:SER:OG	1:A:117:GLU:HG3	1.95	0.67
1:B:9:MET:O	1:B:206:ILE:HA	1.93	0.67
1:C:50:GLU:O	1:C:53:VAL:HG12	1.95	0.67
1:A:20:GLN:HE22	1:A:272:LYS:N	1.88	0.66
1:A:192:GLU:HG3	1:A:243:ILE:HG21	1.75	0.66
1:A:20:GLN:NE2	1:A:271:ARG:HA	2.10	0.66
1:D:163:ALA:HB2	1:D:185:VAL:HB	1.76	0.66
1:A:218:GLN:HA	1:A:218:GLN:NE2	2.06	0.66
1:B:80:VAL:HG13	1:B:91:LEU:HB2	1.78	0.66
1:A:192:GLU:HA	1:A:240:ASN:HD21	1.59	0.65
1:C:286:LYS:O	1:C:290:GLN:HG2	1.96	0.65
1:D:192:GLU:HA	1:D:240:ASN:ND2	2.11	0.65
1:A:213:MET:HE1	1:A:216:ARG:NH1	2.12	0.65
1:B:192:GLU:HG3	1:B:243:ILE:HG21	1.79	0.65
1:C:79:HIS:HE1	1:C:106:VAL:N	1.94	0.65
1:C:282:LEU:O	1:C:286:LYS:HG3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:HD21	1:C:180:GLU:OE2	1.98	0.64
1:D:106:VAL:HG13	1:D:137:TYR:CE2	2.32	0.64
1:B:242:VAL:HG13	1:B:288:LEU:HD21	1.80	0.64
1:D:279:GLU:HA	1:D:282:LEU:HD22	1.80	0.63
1:D:237:THR:HG22	4:D:457:HOH:O	1.98	0.63
1:A:20:GLN:HE21	1:A:271:ARG:HA	1.63	0.63
1:B:148:THR:O	1:B:152:ILE:HG12	1.99	0.63
1:A:80:VAL:CG1	1:A:88:SER:O	2.47	0.63
1:D:108:PRO:HD2	1:D:118:HIS:CD2	2.32	0.63
1:B:279:GLU:HA	1:B:282:LEU:CD2	2.29	0.63
1:C:192:GLU:HG3	1:C:243:ILE:HD13	1.81	0.62
1:C:152:ILE:O	1:C:156:VAL:HG22	1.99	0.62
1:A:213:MET:HE2	1:A:239:CYS:HA	1.80	0.62
1:D:116:GLU:HG3	4:D:771:HOH:O	1.99	0.62
1:B:236:GLN:HE21	1:B:240:ASN:HD21	1.47	0.62
1:C:149:LEU:HD12	1:C:176:GLN:NE2	2.14	0.62
1:D:156:VAL:HA	1:D:161:VAL:HG11	1.80	0.62
1:D:192:GLU:HG3	1:D:243:ILE:HG21	1.82	0.62
1:C:137:TYR:CD1	1:C:165:LYS:HD3	2.35	0.61
1:C:218:GLN:HE21	1:C:218:GLN:CA	2.05	0.61
1:C:249:THR:O	1:C:253:ARG:HD2	1.99	0.61
1:C:243:ILE:O	1:C:247:ILE:HG12	2.00	0.61
1:A:13:LEU:HD13	1:A:48:THR:HG22	1.83	0.61
1:B:83:VAL:HG23	4:B:402:HOH:O	2.00	0.61
1:B:171:LEU:HD12	1:D:171:LEU:HD12	1.82	0.61
1:D:259:LEU:HB3	1:D:265:ILE:HD13	1.83	0.61
1:D:279:GLU:O	1:D:282:LEU:HD22	2.01	0.61
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.66	0.60
1:A:192:GLU:CG	1:A:243:ILE:HG21	2.31	0.60
1:C:167:THR:HA	1:C:189:GLY:HA3	1.84	0.60
1:C:192:GLU:HG3	1:C:243:ILE:HG21	1.83	0.60
1:B:106:VAL:HA	1:B:137:TYR:HB3	1.83	0.60
1:B:236:GLN:HE21	1:B:240:ASN:ND2	2.00	0.59
1:C:229:ILE:HG13	1:C:230:GLN:N	2.18	0.59
1:A:148:THR:OG1	1:A:151:GLN:HG3	2.02	0.59
1:D:139:ILE:HD13	1:D:167:THR:CG2	2.33	0.59
1:C:236:GLN:HE21	1:C:240:ASN:HD21	1.50	0.59
1:D:229:ILE:HD13	1:D:229:ILE:N	2.17	0.59
1:C:5:LEU:HD22	1:C:5:LEU:H	1.67	0.58
1:D:213:MET:HE1	1:D:239:CYS:HA	1.86	0.58
1:A:163:ALA:HB2	1:A:185:VAL:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:HG2	1:C:240:ASN:OD1	2.03	0.58
1:A:137:TYR:CD1	1:A:165:LYS:HD3	2.39	0.58
1:B:76:LEU:HB3	1:B:100:PHE:CD2	2.38	0.58
1:C:236:GLN:HE21	1:C:240:ASN:ND2	2.02	0.57
1:A:70:ALA:HB1	1:A:74:ILE:HD13	1.85	0.57
1:D:29:ARG:HD2	1:D:264:VAL:O	2.03	0.57
1:D:62:VAL:O	1:D:66:VAL:HG12	2.05	0.57
1:D:218:GLN:HE21	1:D:218:GLN:HA	1.69	0.57
1:A:79:HIS:HE1	1:A:106:VAL:N	2.03	0.57
1:B:5:LEU:HD23	1:B:5:LEU:H	1.69	0.57
1:C:80:VAL:CG1	1:C:88:SER:O	2.53	0.57
1:C:149:LEU:HD23	1:C:149:LEU:O	2.05	0.57
1:A:56:LEU:HD21	1:A:87:GLU:HB3	1.87	0.56
1:A:253:ARG:HD3	1:A:277:VAL:HG22	1.87	0.56
1:D:41:GLY:HA2	1:D:74:ILE:HB	1.86	0.56
1:B:113:PHE:CZ	1:C:273:PRO:HG2	2.40	0.56
1:C:288:LEU:O	1:C:292:LEU:HD23	2.05	0.56
1:C:294:GLN:HG3	1:C:294:GLN:O	2.05	0.56
1:D:61:GLN:O	1:D:65:ILE:HG12	2.05	0.56
1:B:259:LEU:HB3	1:B:265:ILE:HG12	1.88	0.56
1:B:108:PRO:HD2	1:B:118:HIS:HD2	1.70	0.56
1:A:192:GLU:HA	1:A:240:ASN:ND2	2.20	0.56
1:C:64:GLU:O	1:C:68:GLU:HG3	2.05	0.56
1:A:70:ALA:HB1	1:A:74:ILE:HD11	1.88	0.56
1:B:218:GLN:HA	1:B:218:GLN:NE2	2.17	0.56
1:C:79:HIS:CE1	1:C:106:VAL:H	2.18	0.56
1:B:9:MET:HG3	1:B:41:GLY:C	2.26	0.55
1:A:213:MET:CE	1:A:239:CYS:HA	2.36	0.55
1:B:262:MET:O	1:B:263:ASP:HB2	2.05	0.55
1:B:139:ILE:HG23	1:B:139:ILE:O	2.06	0.55
1:A:9:MET:O	1:A:206:ILE:HA	2.06	0.55
1:D:212:ILE:HG13	1:D:213:MET:HG2	1.89	0.55
1:A:113:PHE:CZ	1:D:273:PRO:HG2	2.42	0.55
1:C:20:GLN:HE22	1:C:272:LYS:HG2	1.72	0.54
1:D:9:MET:HG3	1:D:41:GLY:C	2.27	0.54
1:D:121:HIS:CE1	1:D:125:ILE:HD11	2.42	0.54
1:A:88:SER:HB3	1:A:125:ILE:HD12	1.88	0.54
1:A:271:ARG:O	1:A:274:PHE:HB2	2.07	0.54
1:D:121:HIS:HE1	4:D:544:HOH:O	1.91	0.54
1:A:293:MET:O	1:A:294:GLN:HB2	2.06	0.54
1:D:48:THR:HA	1:D:252:PHE:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PRO:HG2	1:D:113:PHE:CZ	2.43	0.54
1:D:79:HIS:HE1	1:D:106:VAL:N	2.05	0.54
1:C:4:ASN:HA	4:C:631:HOH:O	2.06	0.53
1:D:192:GLU:CG	1:D:243:ILE:HG21	2.38	0.53
1:C:137:TYR:CE1	1:C:165:LYS:HD3	2.44	0.53
1:B:13:LEU:HD13	1:B:48:THR:HG22	1.90	0.53
1:B:271:ARG:O	1:B:274:PHE:HB2	2.09	0.53
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.90	0.53
1:B:80:VAL:HG11	1:B:88:SER:O	2.08	0.53
1:C:80:VAL:O	1:C:80:VAL:HG12	2.07	0.53
1:B:121:HIS:O	1:B:125:ILE:HG13	2.09	0.53
1:B:163:ALA:HB2	1:B:185:VAL:HB	1.90	0.53
1:A:117:GLU:OE2	1:D:253:ARG:NH2	2.42	0.52
1:C:5:LEU:HD22	1:C:5:LEU:N	2.25	0.52
1:D:180:GLU:HG3	4:D:376:HOH:O	2.09	0.52
1:A:26:SER:HA	1:A:29:ARG:NH1	2.24	0.52
1:A:139:ILE:HD11	1:A:142:LEU:HD22	1.92	0.52
1:A:85:THR:HA	1:A:121:HIS:CE1	2.45	0.52
1:C:148:THR:OG1	1:C:151:GLN:HG3	2.10	0.52
1:C:192:GLU:CD	1:C:192:GLU:H	2.12	0.52
1:D:84:SER:OG	1:D:87:GLU:HG3	2.09	0.52
1:D:163:ALA:CB	1:D:185:VAL:HB	2.40	0.52
1:B:35:ILE:HG12	1:B:74:ILE:HD13	1.91	0.52
1:D:192:GLU:CD	1:D:192:GLU:H	2.13	0.52
1:A:113:PHE:CE1	1:D:273:PRO:HG2	2.44	0.52
1:B:178:ARG:NH2	1:B:203:ASP:OD2	2.43	0.52
1:A:217:TYR:O	1:A:221:VAL:HG23	2.09	0.51
1:B:213:MET:HA	1:B:215:TRP:CZ3	2.44	0.51
1:C:155:LEU:O	1:C:158:LEU:HB2	2.11	0.51
1:C:135:VAL:HG22	1:C:163:ALA:HB3	1.92	0.51
1:A:237:THR:HG22	1:A:241:LYS:HE3	1.93	0.51
1:C:56:LEU:HD11	1:C:87:GLU:CG	2.38	0.51
1:A:79:HIS:CE1	1:A:106:VAL:H	2.27	0.51
1:C:173:GLN:HA	1:C:176:GLN:HE21	1.75	0.51
1:A:13:LEU:HD13	1:A:48:THR:CG2	2.40	0.51
1:D:85:THR:OG1	1:D:121:HIS:HD2	1.93	0.51
1:D:229:ILE:HD13	1:D:229:ILE:H	1.76	0.51
1:A:137:TYR:CE1	1:A:165:LYS:HD3	2.46	0.50
1:B:108:PRO:HD2	1:B:118:HIS:CD2	2.47	0.50
1:C:139:ILE:HG23	1:C:139:ILE:O	2.11	0.50
1:D:37:GLN:OE1	1:D:214:GLY:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:HG3	1:A:243:ILE:HD13	1.93	0.50
1:B:294:GLN:O	1:B:294:GLN:HG3	2.11	0.50
1:C:149:LEU:HD23	1:C:149:LEU:C	2.30	0.50
1:C:30:LEU:HD13	1:C:259:LEU:HD13	1.93	0.50
1:B:80:VAL:CG1	1:B:88:SER:O	2.59	0.50
1:B:55:SER:OG	1:B:58:GLU:HG3	2.11	0.50
1:D:165:LYS:HA	1:D:187:TYR:HB2	1.94	0.50
1:A:103:VAL:HG12	1:A:104:SER:N	2.26	0.50
1:C:33:PHE:O	1:C:37:GLN:HG3	2.12	0.50
1:C:221:VAL:HG13	4:C:496:HOH:O	2.10	0.50
1:C:119:CYS:HB3	1:C:123:ARG:NH1	2.27	0.50
1:B:249:THR:O	1:B:253:ARG:HD2	2.11	0.49
1:A:156:VAL:HG11	1:A:184:LEU:HD22	1.93	0.49
1:C:192:GLU:CG	1:C:243:ILE:HG21	2.42	0.49
1:B:212:ILE:HD12	1:B:292:LEU:HD11	1.95	0.49
1:C:9:MET:O	1:C:206:ILE:HA	2.12	0.49
1:B:113:PHE:CE1	1:C:273:PRO:HG2	2.47	0.49
1:B:267:VAL:CG1	1:B:269:LEU:HD23	2.42	0.49
1:A:213:MET:CE	1:A:216:ARG:HD2	2.39	0.49
1:C:131:GLY:O	1:C:132:LEU:O	2.31	0.49
1:C:79:HIS:CE1	1:C:105:ALA:HA	2.48	0.49
1:D:8:VAL:HG13	1:D:210:TYR:CE2	2.48	0.49
1:D:37:GLN:HG3	1:D:215:TRP:HE3	1.78	0.49
1:B:192:GLU:HB3	1:D:172:TYR:CD1	2.48	0.48
1:D:96:LYS:HD3	1:D:132:LEU:HD13	1.94	0.48
1:A:80:VAL:HG12	1:A:80:VAL:O	2.13	0.48
1:C:80:VAL:HG11	1:C:88:SER:O	2.14	0.48
1:A:51:ALA:HA	1:A:54:GLN:HE21	1.76	0.48
1:A:163:ALA:CB	1:A:185:VAL:HB	2.42	0.48
1:C:132:LEU:HD12	1:C:132:LEU:N	2.29	0.48
1:C:253:ARG:HG3	1:C:254:GLY:N	2.27	0.48
1:B:236:GLN:NE2	1:B:240:ASN:HD21	2.09	0.48
1:A:198:LEU:HA	1:A:202:ALA:HB3	1.95	0.47
1:D:53:VAL:O	1:D:53:VAL:HG13	2.13	0.47
1:A:9:MET:HB2	1:A:206:ILE:HG12	1.95	0.47
1:B:175:GLU:HG2	1:D:240:ASN:OD1	2.15	0.47
1:B:261:TYR:CD2	1:B:286:LYS:HA	2.49	0.47
1:B:229:ILE:C	1:B:229:ILE:HD13	2.35	0.47
1:B:117:GLU:OE2	1:C:253:ARG:NH2	2.45	0.47
1:B:51:ALA:HA	1:B:54:GLN:NE2	2.25	0.47
1:B:80:VAL:HG12	1:B:80:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LYS:HA	1:B:187:TYR:HB2	1.95	0.47
1:C:236:GLN:NE2	1:C:240:ASN:HD21	2.13	0.47
1:C:240:ASN:N	1:C:240:ASN:HD22	2.13	0.47
1:D:13:LEU:HD13	1:D:48:THR:CG2	2.45	0.47
1:D:80:VAL:HB	1:D:91:LEU:HB3	1.96	0.47
1:D:147:LEU:HA	1:D:151:GLN:OE1	2.14	0.47
1:D:261:TYR:CD1	1:D:286:LYS:HE3	2.49	0.47
1:A:78:ALA:HB2	1:A:100:PHE:CD2	2.49	0.47
1:B:13:LEU:HD13	1:B:48:THR:CG2	2.44	0.47
1:C:289:ALA:O	1:C:293:MET:HG3	2.15	0.47
1:A:45:GLY:O	1:A:79:HIS:HD2	1.97	0.47
1:B:240:ASN:HD22	1:B:240:ASN:N	2.12	0.47
1:D:51:ALA:HA	1:D:54:GLN:HE21	1.80	0.47
1:D:85:THR:O	1:D:89:GLN:HG3	2.14	0.47
1:A:122:TYR:O	1:A:126:ILE:HG13	2.14	0.47
1:B:267:VAL:HG12	1:B:269:LEU:HD23	1.97	0.47
1:A:80:VAL:HG11	1:A:88:SER:O	2.16	0.46
1:C:256:LYS:HB3	1:C:268:PRO:HA	1.97	0.46
1:D:79:HIS:HE1	1:D:106:VAL:HG22	1.79	0.46
1:D:9:MET:O	1:D:206:ILE:HA	2.16	0.46
1:A:174:MET:SD	1:A:186:LEU:HD13	2.56	0.46
1:D:229:ILE:H	1:D:229:ILE:CD1	2.29	0.46
1:D:18:GLN:HA	1:D:18:GLN:NE2	2.31	0.46
1:D:64:GLU:O	1:D:68:GLU:HG3	2.16	0.46
1:D:122:TYR:O	1:D:126:ILE:HG13	2.16	0.46
1:A:62:VAL:O	1:A:66:VAL:HG23	2.16	0.46
1:A:240:ASN:OD1	1:C:175:GLU:HG2	2.16	0.46
1:A:192:GLU:HB3	1:C:172:TYR:CD1	2.50	0.46
1:B:59:ARG:O	1:B:63:LEU:HG	2.16	0.45
1:B:70:ALA:O	1:B:71:LYS:C	2.54	0.45
1:B:114:SER:OG	1:B:117:GLU:HG3	2.16	0.45
1:A:106:VAL:HA	1:A:137:TYR:HB3	1.98	0.45
1:A:165:LYS:HA	1:A:187:TYR:HB2	1.97	0.45
1:B:292:LEU:O	1:B:294:GLN:N	2.44	0.45
1:D:192:GLU:HG3	1:D:243:ILE:CD1	2.38	0.45
1:A:22:LEU:HD22	4:A:445:HOH:O	2.15	0.45
1:A:54:GLN:HA	1:A:271:ARG:HH21	1.81	0.45
1:A:139:ILE:HG23	1:A:139:ILE:O	2.15	0.45
1:A:28:ARG:HD3	1:A:69:GLU:OE2	2.17	0.45
1:B:121:HIS:CE1	1:B:125:ILE:HD11	2.51	0.45
1:C:76:LEU:HB3	1:C:100:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HG21	1:C:288:LEU:HD23	1.98	0.45
1:D:230:GLN:CA	1:D:230:GLN:HE21	2.28	0.45
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.79	0.45
1:B:148:THR:HG23	1:B:151:GLN:OE1	2.16	0.45
1:B:229:ILE:HD13	1:B:229:ILE:O	2.16	0.45
1:D:55:SER:OG	1:D:58:GLU:HG3	2.17	0.45
1:B:20:GLN:NE2	1:B:271:ARG:HA	2.32	0.45
1:C:14:THR:HG23	1:C:49:GLY:O	2.16	0.44
1:A:45:GLY:O	1:A:79:HIS:CD2	2.70	0.44
1:A:191:ASP:HB3	1:A:217:TYR:OH	2.16	0.44
1:B:31:VAL:O	1:B:35:ILE:HG13	2.17	0.44
1:C:52:PHE:HZ	1:C:106:VAL:HG21	1.82	0.44
1:C:79:HIS:NE2	1:C:106:VAL:HG22	2.32	0.44
1:D:16:PHE:CE2	1:D:271:ARG:HG3	2.51	0.44
1:D:42:LEU:HG	1:D:74:ILE:HD12	2.00	0.44
1:D:253:ARG:HG3	1:D:254:GLY:N	2.33	0.44
1:D:290:GLN:HE21	1:D:290:GLN:HA	1.82	0.44
1:A:196:SER:HB3	1:C:196:SER:HB3	2.00	0.44
1:D:261:TYR:CE1	1:D:286:LYS:HE3	2.52	0.44
1:C:108:PRO:HD2	1:C:118:HIS:HD2	1.82	0.44
1:D:253:ARG:HG2	4:D:551:HOH:O	2.18	0.44
1:A:59:ARG:O	1:A:63:LEU:HG	2.18	0.44
1:B:90:GLN:HE21	1:B:90:GLN:HB2	1.64	0.44
1:C:173:GLN:O	1:C:177:ILE:HG13	2.17	0.44
1:C:277:VAL:HG12	1:C:278:ASP:N	2.33	0.44
1:C:282:LEU:HD13	1:C:282:LEU:HA	1.58	0.44
1:A:80:VAL:HG11	1:A:92:ALA:N	2.33	0.44
1:B:155:LEU:O	1:B:158:LEU:HB2	2.17	0.44
1:B:163:ALA:CB	1:B:185:VAL:HB	2.48	0.44
1:D:8:VAL:HG12	1:D:39:ILE:HD11	2.00	0.44
1:D:271:ARG:O	1:D:274:PHE:HB2	2.18	0.44
1:A:237:THR:HG23	1:C:179:ARG:HD3	1.99	0.43
1:A:284:GLU:HG3	4:A:769:HOH:O	2.17	0.43
1:D:104:SER:HB2	1:D:135:VAL:HB	2.00	0.43
1:D:79:HIS:CE1	1:D:105:ALA:HA	2.54	0.43
1:A:26:SER:HA	1:A:29:ARG:HH11	1.83	0.43
1:A:139:ILE:CD1	1:A:142:LEU:HD22	2.48	0.43
1:A:218:GLN:HE21	1:A:218:GLN:CA	2.08	0.43
1:A:249:THR:HG22	1:A:281:CYS:SG	2.59	0.43
1:D:139:ILE:HD12	4:D:675:HOH:O	2.17	0.43
1:A:153:TYR:HB2	4:A:629:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:OD1	1:A:19:GLN:N	2.48	0.43
1:C:16:PHE:CE2	1:C:271:ARG:HG3	2.54	0.43
1:C:261:TYR:OH	1:C:282:LEU:HD12	2.18	0.43
1:D:79:HIS:CE1	1:D:106:VAL:H	2.26	0.43
1:D:148:THR:OG1	1:D:151:GLN:HG3	2.18	0.43
1:C:164:LEU:CD2	1:C:166:GLN:HG2	2.48	0.43
1:A:16:PHE:CE2	1:A:271:ARG:HG3	2.54	0.43
1:C:97:ARG:HD2	3:C:647:SO4:O2	2.19	0.43
1:B:32:GLN:NE2	1:B:69:GLU:OE1	2.52	0.42
1:D:229:ILE:N	1:D:229:ILE:CD1	2.81	0.42
1:D:282:LEU:N	1:D:283:PRO:HD2	2.34	0.42
1:C:45:GLY:HA3	4:C:307:HOH:O	2.17	0.42
1:A:273:PRO:HG2	1:D:113:PHE:CE1	2.53	0.42
1:B:291:GLN:HG3	1:B:292:LEU:N	2.33	0.42
1:C:103:VAL:CG1	1:C:104:SER:N	2.83	0.42
1:C:288:LEU:HA	1:C:291:GLN:HG2	2.01	0.42
1:A:267:VAL:CG1	1:A:269:LEU:HD23	2.49	0.42
1:D:102:ALA:HA	1:D:132:LEU:HB3	2.01	0.42
1:D:233:GLN:O	1:D:237:THR:CG2	2.64	0.42
1:D:218:GLN:HA	1:D:218:GLN:NE2	2.33	0.42
1:A:156:VAL:HA	1:A:161:VAL:HG11	2.02	0.42
1:B:253:ARG:HD3	1:B:277:VAL:HG22	2.02	0.42
1:A:88:SER:HB2	1:A:125:ILE:CD1	2.50	0.42
1:B:259:LEU:CB	1:B:265:ILE:HG12	2.49	0.42
1:B:279:GLU:HA	1:B:282:LEU:HD22	2.02	0.42
1:C:70:ALA:O	1:C:71:LYS:C	2.58	0.42
1:D:181:HIS:HE1	4:D:377:HOH:O	2.02	0.42
1:C:51:ALA:HA	1:C:54:GLN:HE21	1.84	0.42
1:C:106:VAL:HG13	1:C:137:TYR:CE2	2.54	0.42
1:C:106:VAL:HA	1:C:137:TYR:HB3	2.01	0.42
1:A:48:THR:HA	1:A:252:PHE:CE1	2.55	0.41
1:B:61:GLN:O	1:B:65:ILE:HD12	2.20	0.41
1:C:163:ALA:HB2	1:C:185:VAL:HB	2.02	0.41
1:D:18:GLN:HA	1:D:18:GLN:HE21	1.84	0.41
1:D:80:VAL:HG11	1:D:92:ALA:HA	2.02	0.41
1:B:92:ALA:O	1:B:95:ALA:HB3	2.20	0.41
1:C:8:VAL:O	1:C:40:ASP:HB2	2.21	0.41
1:D:290:GLN:HA	1:D:290:GLN:NE2	2.35	0.41
1:A:80:VAL:HG12	1:A:88:SER:O	2.20	0.41
1:B:61:GLN:HG2	1:B:65:ILE:CD1	2.50	0.41
1:D:194:PHE:CE2	1:D:198:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ALA:O	1:A:293:MET:HG3	2.20	0.41
1:D:45:GLY:O	1:D:79:HIS:HD2	2.04	0.41
1:A:291:GLN:O	1:A:294:GLN:N	2.54	0.41
1:B:218:GLN:HE21	1:B:218:GLN:CA	2.18	0.41
1:B:245:LEU:O	1:B:249:THR:HG23	2.20	0.41
1:B:287:ALA:O	1:B:290:GLN:HB2	2.19	0.41
1:C:288:LEU:HA	1:C:291:GLN:HE21	1.86	0.41
1:D:4:ASN:N	4:D:318:HOH:O	2.54	0.41
1:D:13:LEU:HD13	1:D:48:THR:HG22	2.02	0.41
1:A:237:THR:O	1:A:241:LYS:HG3	2.20	0.40
1:C:150:GLY:O	1:C:153:TYR:HB3	2.20	0.40
1:D:260:HIS:HD2	1:D:265:ILE:O	2.04	0.40
1:C:25:ALA:HB1	1:C:29:ARG:HH21	1.86	0.40
1:C:249:THR:HG22	1:C:281:CYS:SG	2.61	0.40
1:A:287:ALA:O	1:A:290:GLN:HB2	2.21	0.40
1:D:83:VAL:HG23	4:D:362:HOH:O	2.20	0.40
1:A:229:ILE:O	1:A:233:GLN:HG3	2.21	0.40
1:C:253:ARG:HD3	1:C:277:VAL:HA	2.04	0.40
1:D:97:ARG:HD3	3:D:645:SO4:O2	2.22	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	289/319 (91%)	282 (98%)	7 (2%)	0	100 100
1	B	289/319 (91%)	276 (96%)	13 (4%)	0	100 100
1	C	289/319 (91%)	275 (95%)	12 (4%)	2 (1%)	22 23
1	D	289/319 (91%)	279 (96%)	10 (4%)	0	100 100
All	All	1156/1276 (91%)	1112 (96%)	42 (4%)	2 (0%)	47 56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	LEU
1	C	251	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/261 (91%)	227 (95%)	11 (5%)	27	32
1	B	238/261 (91%)	224 (94%)	14 (6%)	19	22
1	C	238/261 (91%)	231 (97%)	7 (3%)	42	52
1	D	238/261 (91%)	219 (92%)	19 (8%)	12	12
All	All	952/1044 (91%)	901 (95%)	51 (5%)	22	25

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	27	LEU
1	A	44	VAL
1	A	74	ILE
1	A	76	LEU
1	A	91	LEU
1	A	149	LEU
1	A	175	GLU
1	A	203	ASP
1	A	218	GLN
1	A	234	LYS
1	B	5	LEU
1	B	6	ARG
1	B	9	MET
1	B	91	LEU
1	B	103	VAL
1	B	149	LEU
1	B	158	LEU

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Mol	Chain	Res	Type
1	B	175	GLU
1	B	218	GLN
1	B	229	ILE
1	B	234	LYS
1	B	263	ASP
1	B	271	ARG
1	B	282	LEU
1	C	14	THR
1	C	27	LEU
1	C	106	VAL
1	C	115	LEU
1	C	175	GLU
1	C	218	GLN
1	C	282	LEU
1	D	9	MET
1	D	27	LEU
1	D	44	VAL
1	D	53	VAL
1	D	73	LYS
1	D	76	LEU
1	D	91	LEU
1	D	106	VAL
1	D	139	ILE
1	D	149	LEU
1	D	175	GLU
1	D	186	LEU
1	D	218	GLN
1	D	229	ILE
1	D	230	GLN
1	D	237	THR
1	D	263	ASP
1	D	282	LEU
1	D	294	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	18	GLN
1	A	20	GLN
1	A	54	GLN
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	79	HIS
1	A	90	GLN
1	A	118	HIS
1	A	138	ASN
1	A	166	GLN
1	A	218	GLN
1	A	233	GLN
1	A	240	ASN
1	A	260	HIS
1	B	18	GLN
1	B	20	GLN
1	B	37	GLN
1	B	54	GLN
1	B	61	GLN
1	B	90	GLN
1	B	118	HIS
1	B	121	HIS
1	B	138	ASN
1	B	166	GLN
1	B	176	GLN
1	B	218	GLN
1	B	230	GLN
1	B	240	ASN
1	B	260	HIS
1	B	294	GLN
1	C	4	ASN
1	C	18	GLN
1	C	20	GLN
1	C	54	GLN
1	C	61	GLN
1	C	79	HIS
1	C	90	GLN
1	C	118	HIS
1	C	138	ASN
1	C	166	GLN
1	C	176	GLN
1	C	218	GLN
1	C	240	ASN
1	C	260	HIS
1	C	291	GLN
1	C	294	GLN
1	D	18	GLN

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Mol	Chain	Res	Type
1	D	54	GLN
1	D	79	HIS
1	D	90	GLN
1	D	118	HIS
1	D	121	HIS
1	D	138	ASN
1	D	166	GLN
1	D	176	GLN
1	D	181	HIS
1	D	218	GLN
1	D	230	GLN
1	D	240	ASN
1	D	260	HIS
1	D	290	GLN
1	D	294	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	3PY	B	641	1	5,5,6	1.87	1 (20%)	4,5,7	5.98	4 (100%)
3	SO4	B	646	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	C	647	-	4,4,4	0.24	0	6,6,6	0.07	0
2	3PY	C	642	1	5,5,6	1.96	1 (20%)	4,5,7	6.02	3 (75%)
2	3PY	A	640	1	5,5,6	1.93	1 (20%)	4,5,7	5.92	2 (50%)
2	3PY	D	643	1	5,5,6	1.95	1 (20%)	4,5,7	6.03	4 (100%)
3	SO4	D	645	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	A	644	-	4,4,4	0.22	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3PY	D	643	1	-	2/3/3/6	-
2	3PY	C	642	1	-	2/3/3/6	-
2	3PY	A	640	1	-	1/3/3/6	-
2	3PY	B	641	1	-	3/3/3/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	640	3PY	O4-C3	-3.43	1.24	1.42
2	C	642	3PY	O4-C3	-3.41	1.24	1.42
2	D	643	3PY	O4-C3	-3.38	1.24	1.42
2	B	641	3PY	O4-C3	-3.33	1.24	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	642	3PY	O2-C1-C2	8.34	140.84	114.03
2	D	643	3PY	O2-C1-C2	8.34	140.82	114.03
2	B	641	3PY	O2-C1-C2	8.33	140.79	114.03
2	D	643	3PY	O2-C1-O1	-8.21	102.83	123.30
2	C	642	3PY	O2-C1-O1	-8.20	102.86	123.30
2	A	640	3PY	O2-C1-C2	8.18	140.30	114.03
2	A	640	3PY	O2-C1-O1	-8.13	103.03	123.30
2	B	641	3PY	O2-C1-O1	-8.03	103.29	123.30
2	B	641	3PY	O1-C1-C2	-2.23	115.92	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	642	3PY	O1-C1-C2	-2.11	116.30	123.08
2	D	643	3PY	O1-C1-C2	-2.09	116.35	123.08
2	D	643	3PY	O4-C3-C2	-2.06	102.95	111.03
2	B	641	3PY	O4-C3-C2	-2.04	103.04	111.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	640	3PY	C1-C2-C3-O4
2	B	641	3PY	C1-C2-C3-O4
2	D	643	3PY	C1-C2-C3-O4
2	C	642	3PY	O1-C1-C2-C3
2	C	642	3PY	O2-C1-C2-C3
2	B	641	3PY	O2-C1-C2-C3
2	B	641	3PY	O1-C1-C2-C3
2	D	643	3PY	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	647	SO4	1	0
3	D	645	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 (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	291/319 (91%)	-0.14	3 (1%)	82	88	28, 39, 54, 65	16 (5%)
1	B	291/319 (91%)	0.18	15 (5%)	27	39	34, 44, 63, 76	16 (5%)
1	C	291/319 (91%)	0.19	21 (7%)	15	23	30, 48, 65, 86	16 (5%)
1	D	291/319 (91%)	-0.08	3 (1%)	82	88	26, 38, 54, 68	13 (4%)
All	All	1164/1276 (91%)	0.04	42 (3%)	42	55	26, 42, 62, 86	61 (5%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	TYR	3.9
1	C	206	ILE	3.4
1	C	46	GLY	3.2
1	B	11	ALA	3.1
1	B	43	TYR	3.0
1	C	292	LEU	2.9
1	B	227	GLY	2.9
1	B	48	THR	2.9
1	B	135	VAL	2.7
1	C	137	TYR	2.7
1	C	105	ALA	2.6
1	B	10	ALA	2.5
1	B	282	LEU	2.5
1	C	48	THR	2.4
1	D	206	ILE	2.4
1	C	70	ALA	2.4
1	C	72	GLY	2.4
1	C	106	VAL	2.4
1	D	13	LEU	2.4
1	C	290	GLN	2.4
1	C	104	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	72	GLY	2.3
1	C	18	GLN	2.3
1	C	286	LYS	2.3
1	B	12	LEU	2.2
1	C	136	VAL	2.2
1	C	230	GLN	2.2
1	B	148	THR	2.2
1	D	11	ALA	2.2
1	B	208	SER	2.2
1	B	165	LYS	2.2
1	C	80	VAL	2.1
1	A	72	GLY	2.1
1	B	263	ASP	2.1
1	C	294	GLN	2.1
1	C	43	TYR	2.1
1	C	207	GLY	2.1
1	A	11	ALA	2.1
1	C	278	ASP	2.0
1	A	180	GLU	2.0
1	B	77	ILE	2.0
1	C	47	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	3PY	D	643	6/7	0.88	0.45	55,56,59,62	0
3	SO4	B	646	5/5	0.91	0.16	57,57,58,58	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	3PY	A	640	6/7	0.92	0.40	46,50,54,57	0
2	3PY	B	641	6/7	0.93	0.41	52,54,58,61	0
2	3PY	C	642	6/7	0.95	0.39	49,50,56,63	0
3	SO4	C	647	5/5	0.96	0.14	47,49,50,50	5
3	SO4	A	644	5/5	0.98	0.12	42,43,44,46	5
3	SO4	D	645	5/5	0.99	0.09	42,44,45,47	0

6.5 Other polymers (i)

There are no such residues in this entry.