Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 11:33 pm GMT

PDB ID	:	5G0A
Title	:	The crystal structure of a S-selective transaminase from Bacillus megaterium
Authors	:	van Oosterwijk, N.; Willies, S.; Hekelaar, J.; Terwisscha van Scheltinga, A.C.; Turner, N.J.; Dijkstra, B.W.
Deposited on	:	2016-03-17
Resolution	:	1.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

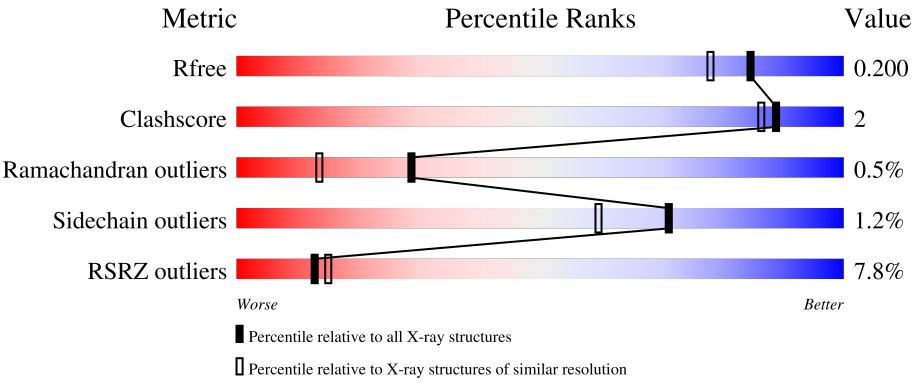
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	483	3% 92% 5% .
1	B	483	11% 91% 7% .
1	C	483	7% 92% 5% .
1	D	483	9% 94% . .

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16190 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 TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	1	0
			3695	2344	624	707	20			
1	B	473	Total	C	N	O	S	0	1	0
			3733	2367	630	717	19			
1	C	468	Total	C	N	O	S	0	0	0
			3687	2339	623	706	19			
1	D	473	Total	C	N	O	S	0	1	0
			3732	2367	630	715	20			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLN	PRO	conflict	UNP A0A0Q9UXH
A	90	ALA	SER	conflict	UNP A0A0Q9UXH
A	202	ASP	ASN	conflict	UNP A0A0Q9UXH
A	205	LEU	CYS	conflict	UNP A0A0Q9UXH
A	268	ASN	THR	conflict	UNP A0A0Q9UXH
A	318	ALA	GLU	conflict	UNP A0A0Q9UXH
A	322	LYS	ARG	conflict	UNP A0A0Q9UXH
A	359	ASP	ASN	conflict	UNP A0A0Q9UXH
A	452	GLY	GLU	conflict	UNP A0A0Q9UXH
A	475	ALA	-	expression tag	UNP A0A0Q9UXH
A	476	LEU	-	expression tag	UNP A0A0Q9UXH
A	477	GLU	-	expression tag	UNP A0A0Q9UXH
A	478	HIS	-	expression tag	UNP A0A0Q9UXH
A	479	HIS	-	expression tag	UNP A0A0Q9UXH
A	480	HIS	-	expression tag	UNP A0A0Q9UXH
A	481	HIS	-	expression tag	UNP A0A0Q9UXH
A	482	HIS	-	expression tag	UNP A0A0Q9UXH
A	483	HIS	-	expression tag	UNP A0A0Q9UXH
B	69	GLN	PRO	conflict	UNP A0A0Q9UXH
B	90	ALA	SER	conflict	UNP A0A0Q9UXH
B	202	ASP	ASN	conflict	UNP A0A0Q9UXH

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Chain	Residue	Modelled	Actual	Comment	Reference
B	205	LEU	CYS	conflict	UNP A0A0Q9UXH
B	268	ASN	THR	conflict	UNP A0A0Q9UXH
B	318	ALA	GLU	conflict	UNP A0A0Q9UXH
B	322	LYS	ARG	conflict	UNP A0A0Q9UXH
B	359	ASP	ASN	conflict	UNP A0A0Q9UXH
B	452	GLY	GLU	conflict	UNP A0A0Q9UXH
B	475	ALA	-	expression tag	UNP A0A0Q9UXH
B	476	LEU	-	expression tag	UNP A0A0Q9UXH
B	477	GLU	-	expression tag	UNP A0A0Q9UXH
B	478	HIS	-	expression tag	UNP A0A0Q9UXH
B	479	HIS	-	expression tag	UNP A0A0Q9UXH
B	480	HIS	-	expression tag	UNP A0A0Q9UXH
B	481	HIS	-	expression tag	UNP A0A0Q9UXH
B	482	HIS	-	expression tag	UNP A0A0Q9UXH
B	483	HIS	-	expression tag	UNP A0A0Q9UXH
C	69	GLN	PRO	conflict	UNP A0A0Q9UXH
C	90	ALA	SER	conflict	UNP A0A0Q9UXH
C	202	ASP	ASN	conflict	UNP A0A0Q9UXH
C	205	LEU	CYS	conflict	UNP A0A0Q9UXH
C	268	ASN	THR	conflict	UNP A0A0Q9UXH
C	318	ALA	GLU	conflict	UNP A0A0Q9UXH
C	322	LYS	ARG	conflict	UNP A0A0Q9UXH
C	359	ASP	ASN	conflict	UNP A0A0Q9UXH
C	452	GLY	GLU	conflict	UNP A0A0Q9UXH
C	475	ALA	-	expression tag	UNP A0A0Q9UXH
C	476	LEU	-	expression tag	UNP A0A0Q9UXH
C	477	GLU	-	expression tag	UNP A0A0Q9UXH
C	478	HIS	-	expression tag	UNP A0A0Q9UXH
C	479	HIS	-	expression tag	UNP A0A0Q9UXH
C	480	HIS	-	expression tag	UNP A0A0Q9UXH
C	481	HIS	-	expression tag	UNP A0A0Q9UXH
C	482	HIS	-	expression tag	UNP A0A0Q9UXH
C	483	HIS	-	expression tag	UNP A0A0Q9UXH
D	69	GLN	PRO	conflict	UNP A0A0Q9UXH
D	90	ALA	SER	conflict	UNP A0A0Q9UXH
D	202	ASP	ASN	conflict	UNP A0A0Q9UXH
D	205	LEU	CYS	conflict	UNP A0A0Q9UXH
D	268	ASN	THR	conflict	UNP A0A0Q9UXH
D	318	ALA	GLU	conflict	UNP A0A0Q9UXH
D	322	LYS	ARG	conflict	UNP A0A0Q9UXH
D	359	ASP	ASN	conflict	UNP A0A0Q9UXH
D	452	GLY	GLU	conflict	UNP A0A0Q9UXH

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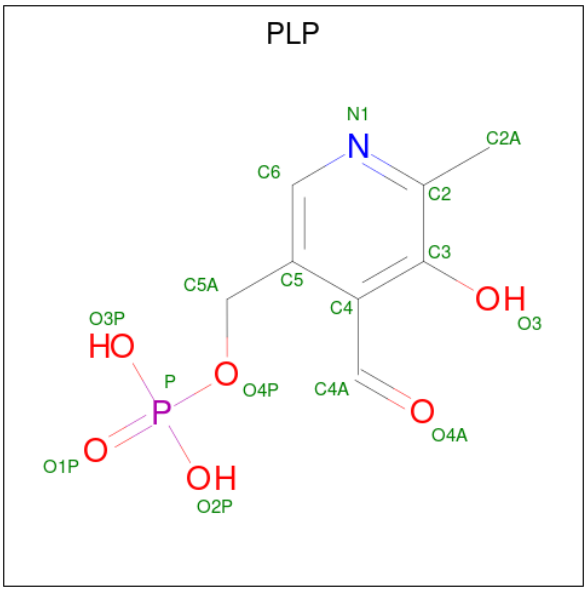
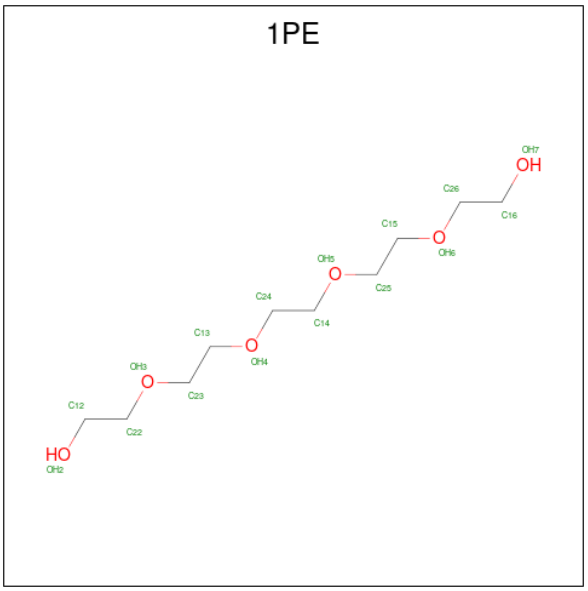
Chain	Residue	Modelled	Actual	Comment	Reference
D	475	ALA	-	expression tag	UNP A0A0Q9UXH
D	476	LEU	-	expression tag	UNP A0A0Q9UXH
D	477	GLU	-	expression tag	UNP A0A0Q9UXH
D	478	HIS	-	expression tag	UNP A0A0Q9UXH
D	479	HIS	-	expression tag	UNP A0A0Q9UXH
D	480	HIS	-	expression tag	UNP A0A0Q9UXH
D	481	HIS	-	expression tag	UNP A0A0Q9UXH
D	482	HIS	-	expression tag	UNP A0A0Q9UXH
D	483	HIS	-	expression tag	UNP A0A0Q9UXH

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



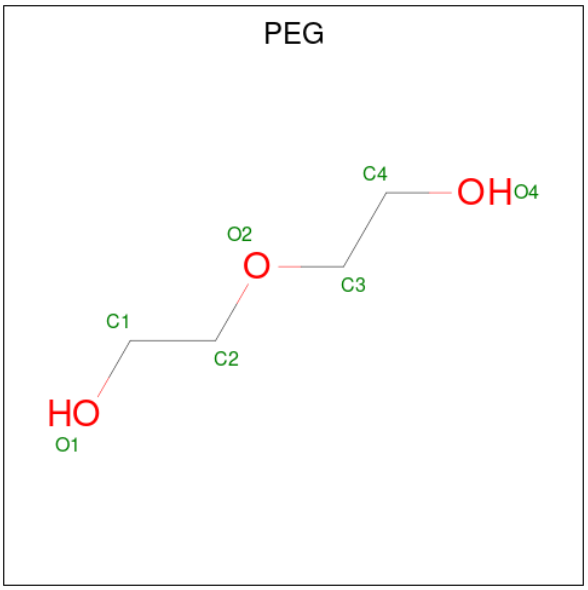
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



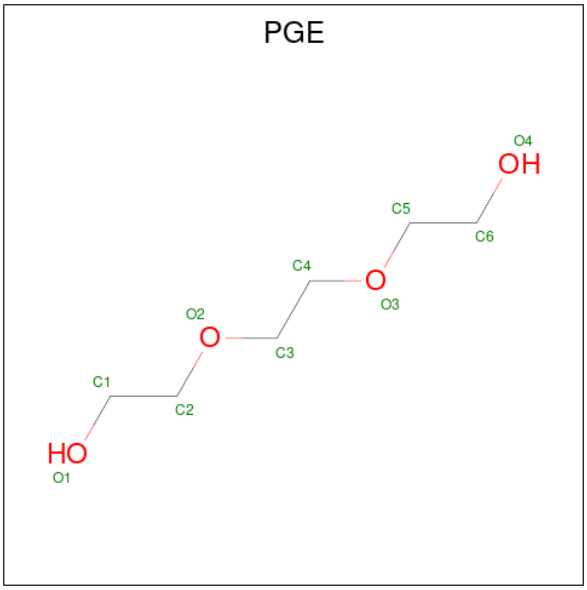
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



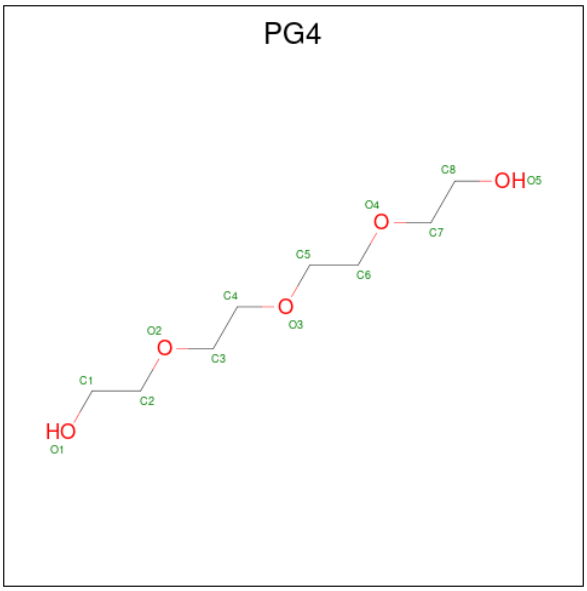
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	D	1	Total C O 10 6 4	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 13 8 5	0	0
6	C	1	Total C O 13 8 5	0	0
6	C	1	Total C O 13 8 5	0	0
6	C	1	Total C O 13 8 5	0	0
6	C	1	Total C O 13 8 5	0	0

- Molecule 7 is water.

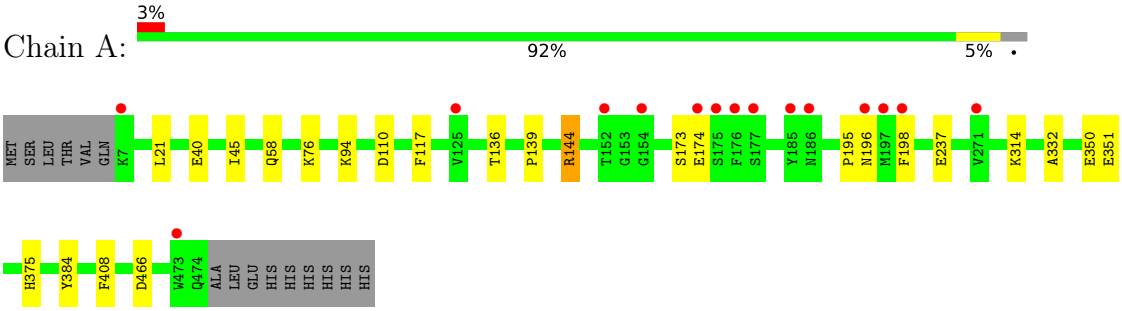
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	371	Total O 371 371	0	0
7	B	236	Total O 236 236	0	0
7	C	285	Total O 285 285	0	0
7	D	204	Total O 204 204	0	0

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.

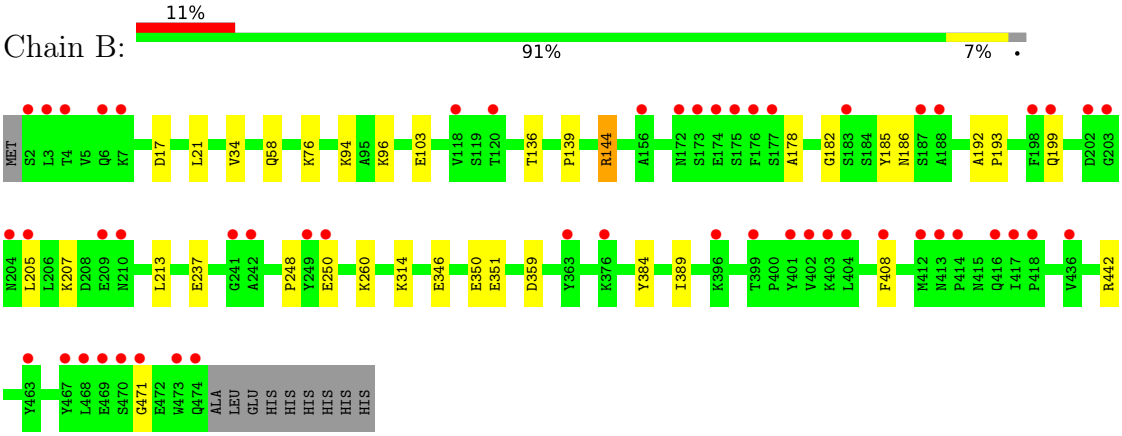
• Molecule 1: TRANSAMINASE

Chain A:



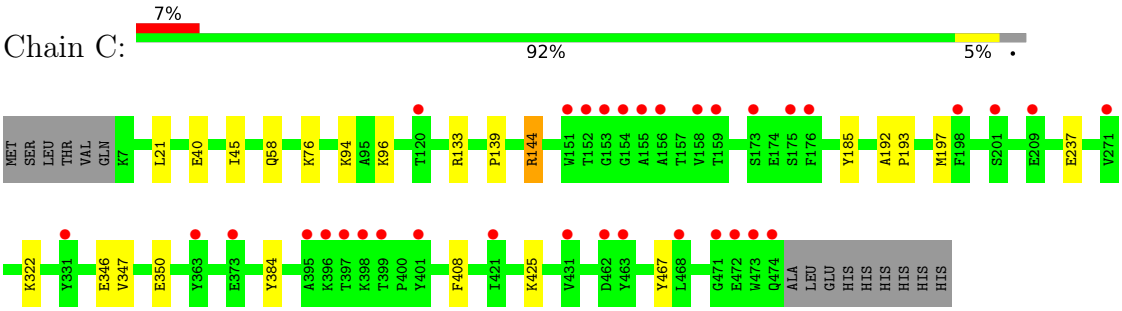
• Molecule 1: TRANSAMINASE

Chain B:



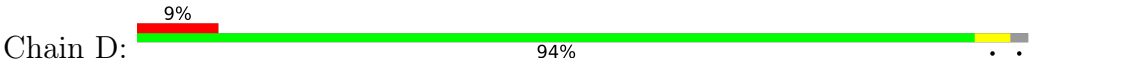
• Molecule 1: TRANSAMINASE

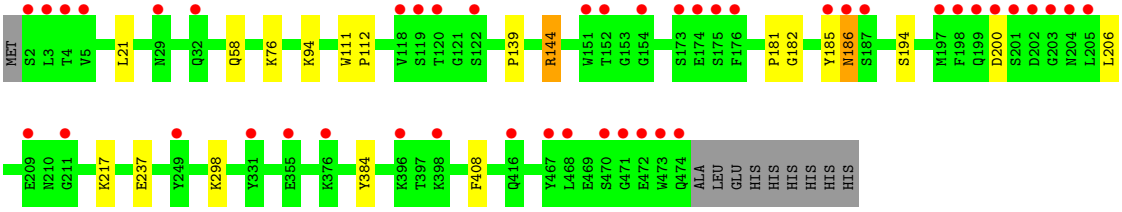
Chain C:



• Molecule 1: TRANSAMINASE

Chain D:




MET
S2
L3
T4
V5
L21
N29
Q32
Q58
K76
K94
W111
P112
V118
S119
T120
G121
S122
P139
R144
W151
T152
G153
G154
S173
E174
S175
F176
P181
G182
Y185
N186
S187
S194
M197
F198
Q199
D200
S201
D202
G203
N204
L205
L206
E209
N210
G211
K217
E237
Y249
K298
Y331
E355
K376
Y384
K396
T397
K398
F408
Q416
Y467
L468
E469
S470
G471
E472
W473
Q474
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.14Å 124.64Å 126.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.42 – 1.70 43.42 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (43.42-1.70) 96.6 (43.42-1.70)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.172 , 0.200 0.173 , 0.200	Depositor DCC
R_{free} test set	9934 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16190	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PLP, PEG, PG4, 1PE

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	0.54	0/3776	0.65	0/5114
1	B	0.50	0/3814	0.65	0/5167
1	C	0.47	0/3768	0.63	0/5104
1	D	0.49	0/3813	0.63	0/5165
All	All	0.50	0/15171	0.64	0/20550

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

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	3695	0	3630	13	0
1	B	3733	0	3667	23	0
1	C	3687	0	3622	14	0
1	D	3732	0	3670	12	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
3	A	48	0	66	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	16	0	22	2	0
4	A	7	0	10	0	0
4	B	14	0	20	2	0
4	C	7	0	10	0	0
5	A	10	0	14	2	0
5	B	10	0	14	4	0
5	D	10	0	14	0	0
6	B	13	0	18	1	0
6	C	52	0	72	0	0
7	A	371	0	0	3	0
7	B	236	0	0	3	0
7	C	285	0	0	3	0
7	D	204	0	0	0	0
All	All	16190	0	14873	58	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 2.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HG2	1:A:45:ILE:HD11	1.67	0.74
1:C:21:LEU:HD13	1:D:94:LYS:HE3	1.72	0.70
1:B:96:LYS:CE	1:B:346:GLU:OE2	2.41	0.68
1:B:182:GLY:HA2	1:B:185:TYR:CE1	2.33	0.63
1:D:182:GLY:HA2	1:D:185:TYR:CD1	2.35	0.61
1:C:94:LYS:HE3	1:D:21:LEU:HD13	1.82	0.60
1:A:21:LEU:HD13	1:B:94:LYS:HE3	1.83	0.59
5:B:1476:PGE:H1	7:B:2106:HOH:O	2.01	0.59
1:B:34:VAL:HG21	6:B:1478:PG4:H81	1.85	0.58
7:A:2150:HOH:O	1:B:178:ALA:HB1	2.04	0.57
1:B:182:GLY:HA2	1:B:185:TYR:CD1	2.39	0.57
1:C:40:GLU:HG2	1:C:45:ILE:HD11	1.86	0.57
1:A:76:LYS:HG2	1:B:76:LYS:HG2	1.87	0.55
1:A:94:LYS:HE3	1:B:21:LEU:HD13	1.89	0.55
5:B:1476:PGE:H52	7:B:2106:HOH:O	2.08	0.54
1:A:136:THR:HG22	5:A:1479:PGE:H42	1.91	0.53
1:B:260:LYS:HZ1	4:B:1477:PEG:H22	1.73	0.53
1:C:185:TYR:O	1:D:186:ASN:OD1	2.28	0.52
1:C:322:LYS:HE2	7:C:2235:HOH:O	2.10	0.52
1:B:96:LYS:NZ	1:B:346:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:CD1	1:D:94:LYS:HE3	2.41	0.51
1:B:199:GLN:HG2	1:B:205:LEU:HD13	1.94	0.50
1:B:17:ASP:HA	1:B:21:LEU:HD12	1.94	0.50
1:B:260:LYS:NZ	4:B:1477:PEG:H22	2.27	0.50
1:B:103[A]:GLU:HA	1:B:103[A]:GLU:OE1	2.13	0.49
1:D:182:GLY:HA2	1:D:185:TYR:CE1	2.48	0.49
1:D:200:ASP:HB3	1:D:206:LEU:HD21	1.93	0.49
7:C:2085:HOH:O	3:D:1475:1PE:H241	2.13	0.49
1:B:350:GLU:HG2	1:B:351:GLU:HG3	1.93	0.48
1:B:389:ILE:HG23	1:B:442:ARG:NH1	2.30	0.47
1:A:198:PHE:CE1	1:D:217:LYS:HD3	2.50	0.46
5:A:1479:PGE:H6	7:A:2146:HOH:O	2.16	0.46
1:C:76:LYS:HG2	1:D:76:LYS:HG2	1.98	0.45
1:C:425:LYS:HG3	1:C:467:TYR:CD2	2.52	0.45
1:B:136:THR:HG22	5:B:1476:PGE:H3	1.98	0.45
7:C:2249:HOH:O	3:D:1475:1PE:H162	2.17	0.45
1:C:192:ALA:HB1	1:C:193:PRO:HD2	1.99	0.44
1:B:314:LYS:NZ	7:B:2089:HOH:O	2.35	0.44
1:A:173:SER:OG	1:A:174:GLU:N	2.51	0.43
1:C:347:VAL:HA	1:C:350:GLU:HG2	2.01	0.43
1:D:144:ARG:NH2	1:D:237:GLU:H	2.16	0.43
1:D:111:TRP:CD1	1:D:112:PRO:HD3	2.54	0.43
1:B:144:ARG:NH2	1:B:237:GLU:H	2.17	0.42
1:B:205:LEU:HG	1:B:248:PRO:HG3	2.01	0.42
1:C:144:ARG:NH2	1:C:237:GLU:H	2.17	0.42
1:C:96:LYS:HE2	1:C:346:GLU:OE2	2.18	0.42
1:A:195:PRO:O	1:A:196:ASN:HB2	2.18	0.42
1:C:425:LYS:HE3	1:C:467:TYR:CD1	2.55	0.42
1:B:192:ALA:HB1	1:B:193:PRO:HD2	2.01	0.42
1:A:314:LYS:NZ	7:A:2120:HOH:O	2.41	0.42
1:B:96:LYS:HE3	1:B:346:GLU:OE2	2.16	0.42
5:B:1476:PGE:H1	5:B:1476:PGE:H32	1.86	0.42
1:C:133:ARG:HB3	1:D:181:PRO:HD2	2.03	0.41
1:A:375:HIS:HE1	1:A:466:ASP:OD1	2.04	0.41
1:B:207:LYS:HG2	1:B:213:LEU:HD23	2.03	0.41
1:A:350:GLU:HG3	1:A:351:GLU:HG3	2.03	0.41
1:A:117:PHE:O	1:A:332:ALA:HB1	2.21	0.40
1:A:144:ARG:NH2	1:A:237:GLU:H	2.19	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	467/483 (97%)	453 (97%)	12 (3%)	2 (0%)	34	18
1	B	472/483 (98%)	451 (96%)	18 (4%)	3 (1%)	25	11
1	C	466/483 (96%)	451 (97%)	13 (3%)	2 (0%)	34	18
1	D	472/483 (98%)	454 (96%)	15 (3%)	3 (1%)	25	11
All	All	1877/1932 (97%)	1809 (96%)	58 (3%)	10 (0%)	29	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	471	GLY
1	A	58	GLN
1	B	58	GLN
1	C	58	GLN
1	D	58	GLN
1	D	298	LYS
1	B	139	PRO
1	D	139	PRO
1	C	139	PRO
1	A	139	PRO

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	395/408 (97%)	391 (99%)	4 (1%)	76	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	400/408 (98%)	394 (98%)	6 (2%)	65 51
1	C	394/408 (97%)	390 (99%)	4 (1%)	76 67
1	D	400/408 (98%)	395 (99%)	5 (1%)	69 56
All	All	1589/1632 (97%)	1570 (99%)	19 (1%)	71 59

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	144	ARG
1	A	384	TYR
1	A	408	PHE
1	B	144	ARG
1	B	186	ASN
1	B	250	GLU
1	B	359	ASP
1	B	384	TYR
1	B	408	PHE
1	C	144	ARG
1	C	197	MET
1	C	384	TYR
1	C	408	PHE
1	D	144	ARG
1	D	186	ASN
1	D	194	SER
1	D	384	TYR
1	D	408	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	268	ASN
1	B	268	ASN
1	C	268	ASN
1	D	268	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

20 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	$\#\|Z\| > 2$
6	PG4	B	1478	-	12,12,12	0.40	0	11,11,11	0.38	0
4	PEG	C	1475	-	6,6,6	0.48	0	5,5,5	0.31	0
2	PLP	C	1298	1	15,15,16	2.94	3 (20%)	20,22,23	1.64	4 (20%)
3	1PE	A	1475	-	15,15,15	0.53	0	14,14,14	0.32	0
4	PEG	B	1477	-	6,6,6	0.55	0	5,5,5	0.39	0
5	PGE	D	1476	-	9,9,9	0.43	0	8,8,8	0.30	0
5	PGE	A	1479	-	9,9,9	0.47	0	8,8,8	0.57	0
2	PLP	D	1298	1	15,15,16	2.82	3 (20%)	20,22,23	1.60	4 (20%)
3	1PE	D	1475	-	15,15,15	0.47	0	14,14,14	0.35	0
3	1PE	A	1476	-	15,15,15	0.46	0	14,14,14	0.33	0
3	1PE	A	1478	-	15,15,15	0.48	0	14,14,14	0.32	0
2	PLP	A	1298	1	15,15,16	2.53	3 (20%)	20,22,23	1.53	4 (20%)
6	PG4	C	1479	-	12,12,12	0.48	0	11,11,11	0.29	0
2	PLP	B	1298	1	15,15,16	3.01	3 (20%)	20,22,23	1.66	6 (30%)
6	PG4	C	1476	-	12,12,12	0.42	0	11,11,11	0.40	0
6	PG4	C	1478	-	12,12,12	0.41	0	11,11,11	0.48	0
4	PEG	A	1477	-	6,6,6	0.46	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PEG	B	1475	-	6,6,6	0.41	0	5,5,5	0.34	0
6	PG4	C	1477	-	12,12,12	0.51	0	11,11,11	0.40	0
5	PGE	B	1476	-	9,9,9	0.45	0	8,8,8	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	B	1478	-	-	3/10/10/10	-
4	PEG	C	1475	-	-	1/4/4/4	-
2	PLP	C	1298	1	-	0/6/6/8	0/1/1/1
3	1PE	A	1475	-	-	3/13/13/13	-
4	PEG	B	1477	-	-	2/4/4/4	-
5	PGE	D	1476	-	-	1/7/7/7	-
5	PGE	A	1479	-	-	2/7/7/7	-
2	PLP	D	1298	1	-	0/6/6/8	0/1/1/1
3	1PE	D	1475	-	-	6/13/13/13	-
3	1PE	A	1476	-	-	4/13/13/13	-
3	1PE	A	1478	-	-	8/13/13/13	-
2	PLP	A	1298	1	-	0/6/6/8	0/1/1/1
6	PG4	C	1479	-	-	1/10/10/10	-
2	PLP	B	1298	1	-	0/6/6/8	0/1/1/1
6	PG4	C	1476	-	-	4/10/10/10	-
6	PG4	C	1478	-	-	0/10/10/10	-
4	PEG	A	1477	-	-	1/4/4/4	-
4	PEG	B	1475	-	-	2/4/4/4	-
6	PG4	C	1477	-	-	3/10/10/10	-
5	PGE	B	1476	-	-	0/7/7/7	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1298	PLP	C5-C4	8.40	1.49	1.40
2	B	1298	PLP	C3-C2	7.73	1.48	1.40
2	B	1298	PLP	C5-C4	7.47	1.48	1.40
2	D	1298	PLP	C5-C4	7.39	1.48	1.40
2	D	1298	PLP	C3-C2	6.73	1.47	1.40
2	A	1298	PLP	C5-C4	6.54	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1298	PLP	C3-C2	6.20	1.47	1.40
2	A	1298	PLP	C3-C2	5.51	1.46	1.40
2	A	1298	PLP	C3-C4	3.87	1.48	1.40
2	C	1298	PLP	C3-C4	3.71	1.47	1.40
2	D	1298	PLP	C3-C4	3.67	1.47	1.40
2	B	1298	PLP	C3-C4	3.57	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1298	PLP	C6-N1-C2	3.37	125.41	119.17
2	B	1298	PLP	C4A-C4-C5	3.11	124.14	120.94
2	B	1298	PLP	C6-C5-C4	2.95	120.48	118.16
2	B	1298	PLP	C3-C4-C5	-2.88	115.63	118.74
2	A	1298	PLP	C6-N1-C2	2.74	124.24	119.17
2	D	1298	PLP	O4P-C5A-C5	2.74	114.57	109.35
2	A	1298	PLP	O4P-C5A-C5	2.63	114.36	109.35
2	D	1298	PLP	C4A-C4-C5	2.61	123.63	120.94
2	D	1298	PLP	C2A-C2-N1	2.58	122.71	117.67
2	D	1298	PLP	C6-N1-C2	2.55	123.88	119.17
2	B	1298	PLP	O4P-P-O1P	-2.34	99.92	106.47
2	B	1298	PLP	O4P-C5A-C5	2.33	113.80	109.35
2	C	1298	PLP	C4A-C4-C5	2.32	123.32	120.94
2	B	1298	PLP	O3-C3-C2	2.14	122.15	117.49
2	A	1298	PLP	C2A-C2-N1	2.07	121.72	117.67
2	A	1298	PLP	C4A-C4-C5	2.06	123.06	120.94
2	C	1298	PLP	C2A-C2-N1	2.04	121.66	117.67
2	C	1298	PLP	C6-C5-C4	2.02	119.75	118.16

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1478	1PE	OH6-C15-C25-OH5
3	A	1478	1PE	OH4-C13-C23-OH3
6	C	1476	PG4	O3-C5-C6-O4
3	A	1478	1PE	OH5-C14-C24-OH4
4	A	1477	PEG	O2-C3-C4-O4
4	B	1477	PEG	O1-C1-C2-O2
3	D	1475	1PE	OH6-C15-C25-OH5
5	A	1479	PGE	O2-C3-C4-O3
3	D	1475	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
4	B	1475	PEG	O1-C1-C2-O2
4	B	1475	PEG	O2-C3-C4-O4
4	B	1477	PEG	O2-C3-C4-O4
6	C	1476	PG4	O4-C7-C8-O5
6	B	1478	PG4	O1-C1-C2-O2
3	A	1478	1PE	OH2-C12-C22-OH3
3	A	1476	1PE	OH5-C14-C24-OH4
3	A	1475	1PE	OH2-C12-C22-OH3
3	D	1475	1PE	C13-C23-OH3-C22
6	B	1478	PG4	C8-C7-O4-C6
5	A	1479	PGE	C4-C3-O2-C2
3	D	1475	1PE	C16-C26-OH6-C15
6	B	1478	PG4	O2-C3-C4-O3
6	C	1477	PG4	C1-C2-O2-C3
6	C	1476	PG4	C4-C3-O2-C2
3	A	1478	1PE	C24-C14-OH5-C25
6	C	1476	PG4	C5-C6-O4-C7
3	A	1476	1PE	C13-C23-OH3-C22
3	A	1478	1PE	C13-C23-OH3-C22
3	A	1478	1PE	C16-C26-OH6-C15
6	C	1479	PG4	O2-C3-C4-O3
3	A	1476	1PE	C16-C26-OH6-C15
3	D	1475	1PE	OH2-C12-C22-OH3
5	D	1476	PGE	O3-C5-C6-O4
6	C	1477	PG4	O4-C7-C8-O5
3	A	1476	1PE	OH4-C13-C23-OH3
3	A	1478	1PE	C15-C25-OH5-C14
3	A	1475	1PE	C12-C22-OH3-C23
6	C	1477	PG4	O3-C5-C6-O4
4	C	1475	PEG	C4-C3-O2-C2
3	A	1475	1PE	OH5-C14-C24-OH4
3	D	1475	1PE	OH4-C13-C23-OH3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1478	PG4	1	0
4	B	1477	PEG	2	0
5	A	1479	PGE	2	0
3	D	1475	1PE	2	0
5	B	1476	PGE	4	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, 95^{th} 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	468/483 (96%)	0.11	15 (3%) 47 52	20, 28, 41, 57	0
1	B	473/483 (97%)	0.66	53 (11%) 5 6	20, 30, 57, 83	0
1	C	468/483 (96%)	0.42	34 (7%) 15 17	22, 32, 51, 78	0
1	D	473/483 (97%)	0.47	45 (9%) 8 9	22, 31, 53, 71	0
All	All	1882/1932 (97%)	0.42	147 (7%) 13 15	20, 30, 52, 83	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	PHE	14.2
1	D	3	LEU	10.2
1	D	201	SER	8.7
1	B	471	GLY	8.2
1	B	3	LEU	7.5
1	D	176	PHE	7.4
1	D	4	THR	7.2
1	B	175	SER	7.0
1	D	473	TRP	6.7
1	A	176	PHE	6.3
1	C	471	GLY	6.3
1	B	174	GLU	6.3
1	C	176	PHE	6.1
1	A	198	PHE	5.7
1	B	474	GLN	5.4
1	B	473	TRP	5.4
1	D	205	LEU	5.4
1	C	396	LYS	5.3
1	D	202	ASP	5.2
1	A	175	SER	5.1
1	D	203	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	198	PHE	5.1
1	B	210	ASN	4.9
1	D	198	PHE	4.9
1	D	471	GLY	4.9
1	C	473	TRP	4.6
1	C	175	SER	4.5
1	B	2	SER	4.4
1	B	468	LEU	4.4
1	B	209	GLU	4.3
1	B	6	GLN	4.2
1	D	5	VAL	4.0
1	B	7	LYS	4.0
1	D	204	ASN	4.0
1	D	249	TYR	3.8
1	B	412	MET	3.8
1	B	414	PRO	3.8
1	D	416	GLN	3.6
1	B	4	THR	3.6
1	B	417	ILE	3.6
1	C	151	TRP	3.4
1	B	183	SER	3.4
1	B	416	GLN	3.3
1	D	32	GLN	3.3
1	B	401	TYR	3.3
1	D	200	ASP	3.3
1	C	397	THR	3.3
1	B	177	SER	3.2
1	C	395	ALA	3.2
1	D	474	GLN	3.2
1	B	203	GLY	3.2
1	D	187	SER	3.1
1	B	418	PRO	3.1
1	B	402	VAL	3.1
1	D	199	GLN	3.0
1	B	413	ASN	2.9
1	C	156	ALA	2.9
1	B	202	ASP	2.9
1	D	118	VAL	2.9
1	B	242	ALA	2.9
1	C	398	LYS	2.9
1	A	197	MET	2.9
1	B	470	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	2	SER	2.9
1	D	186	ASN	2.8
1	B	173	SER	2.8
1	B	403	LYS	2.8
1	B	172	ASN	2.8
1	C	271	VAL	2.8
1	B	467	TYR	2.7
1	D	209	GLU	2.7
1	D	173	SER	2.7
1	D	396	LYS	2.7
1	B	250	GLU	2.7
1	C	472	GLU	2.7
1	B	204	ASN	2.7
1	D	152	THR	2.7
1	D	175	SER	2.7
1	A	7	LYS	2.6
1	A	196	ASN	2.6
1	B	187	SER	2.6
1	C	399	THR	2.6
1	C	463	TYR	2.6
1	B	376	LYS	2.6
1	D	185	TYR	2.6
1	B	399	THR	2.5
1	B	205	LEU	2.5
1	B	118	VAL	2.5
1	C	153	GLY	2.5
1	B	241	GLY	2.5
1	D	29	ASN	2.4
1	C	331	TYR	2.4
1	C	120	THR	2.4
1	D	398	LYS	2.4
1	D	197	MET	2.4
1	D	174	GLU	2.4
1	C	158	VAL	2.4
1	C	468	LEU	2.4
1	C	201	SER	2.4
1	D	376	LYS	2.4
1	B	404	LEU	2.3
1	C	401	TYR	2.3
1	D	472	GLU	2.3
1	B	120	THR	2.3
1	B	396	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	363	TYR	2.3
1	C	159	THR	2.3
1	D	151	TRP	2.3
1	C	431	VAL	2.3
1	B	249	TYR	2.3
1	B	469	GLU	2.3
1	C	209	GLU	2.3
1	B	463	TYR	2.3
1	D	154	GLY	2.3
1	A	186	ASN	2.3
1	D	120	THR	2.2
1	D	468	LEU	2.2
1	B	156	ALA	2.2
1	C	155	ALA	2.2
1	C	154	GLY	2.2
1	A	473	TRP	2.2
1	A	185	TYR	2.2
1	D	331	TYR	2.2
1	C	152	THR	2.2
1	B	436	VAL	2.2
1	C	421	ILE	2.2
1	B	198	PHE	2.1
1	B	363	TYR	2.1
1	B	408	PHE	2.1
1	B	199	GLN	2.1
1	C	474	GLN	2.1
1	D	355	GLU	2.1
1	C	462	ASP	2.1
1	C	373	GLU	2.1
1	D	119	SER	2.1
1	D	122	SER	2.1
1	A	152	THR	2.1
1	A	154	GLY	2.1
1	D	470	SER	2.1
1	D	467	TYR	2.1
1	A	125	VAL	2.1
1	A	271	VAL	2.1
1	B	188	ALA	2.0
1	D	211	GLY	2.0
1	A	177	SER	2.0
1	C	173	SER	2.0
1	A	174	GLU	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, 95^{th} 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
3	1PE	A	1478	16/16	0.76	0.19	49,53,56,56	0
4	PEG	A	1477	7/7	0.79	0.26	51,53,57,62	0
4	PEG	B	1475	7/7	0.79	0.12	56,58,59,60	0
4	PEG	B	1477	7/7	0.80	0.15	43,45,49,50	0
3	1PE	D	1475	16/16	0.82	0.17	44,50,57,60	0
4	PEG	C	1475	7/7	0.82	0.22	47,49,52,56	0
5	PGE	A	1479	10/10	0.83	0.15	40,45,50,51	0
6	PG4	C	1476	13/13	0.83	0.15	52,54,57,61	0
6	PG4	C	1479	13/13	0.83	0.23	50,56,58,60	0
5	PGE	B	1476	10/10	0.86	0.16	33,38,43,45	0
6	PG4	B	1478	13/13	0.86	0.13	45,51,68,71	0
5	PGE	D	1476	10/10	0.87	0.23	43,47,49,53	0
6	PG4	C	1477	13/13	0.87	0.15	40,43,51,52	0
3	1PE	A	1475	16/16	0.87	0.14	35,38,52,54	0
3	1PE	A	1476	16/16	0.88	0.20	40,49,54,54	0
6	PG4	C	1478	13/13	0.89	0.21	38,41,47,51	0
2	PLP	A	1298	15/16	0.97	0.14	20,23,27,28	0
2	PLP	B	1298	15/16	0.97	0.12	22,23,27,30	0
2	PLP	C	1298	15/16	0.97	0.15	23,25,28,31	0
2	PLP	D	1298	15/16	0.97	0.13	24,25,28,31	0

6.5 Other polymers (i)

There are no such residues in this entry.