Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 08:57 am BST

PDB ID	:	4B9B
Title	:	The structure of the omega aminotransferase from Pseudomonas aeruginosa
Authors	:	Sayer, C.; Isupov, M.N.; Westlake, A.; Littlechild, J.A.
Deposited on	:	2012-09-03
Resolution	:	1.64 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:

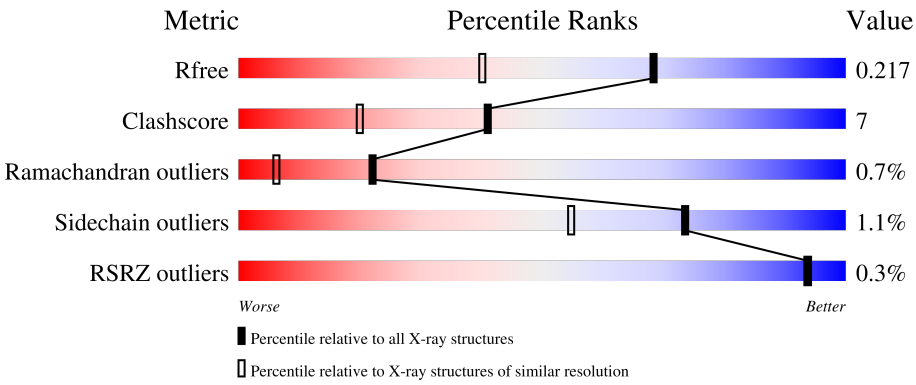
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	448	85% 11% • •
1	B	448	88% 9% •
1	C	448	87% 10% • •
1	D	448	84% 12% • •
1	E	448	88% 9% •

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Mol	Chain	Length	Quality of chain
1	F	448	87% 9%
1	G	448	87% 9%
1	H	448	% 86% 11%

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	PLP	A	500	-	-	X	-
2	PLP	D	500	-	X	-	-
3	GOL	C	504	-	-	X	-

2 Entry composition (i)

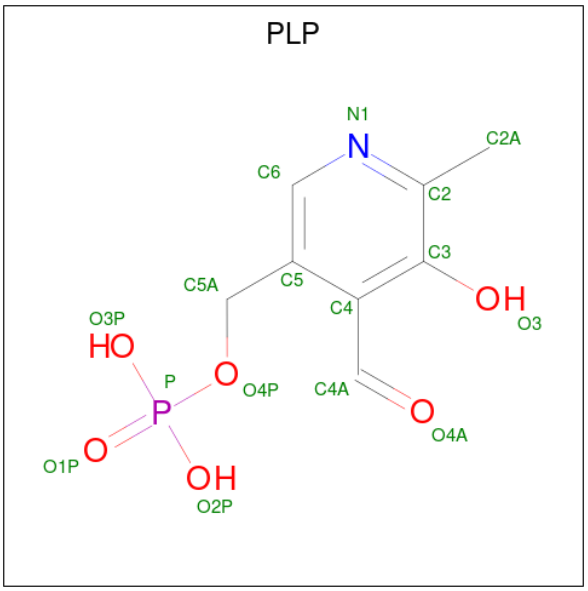
There are 6 unique types of molecules in this entry. The entry contains 33210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-ALANINE-PYRUVATE TRANSAMINASE.

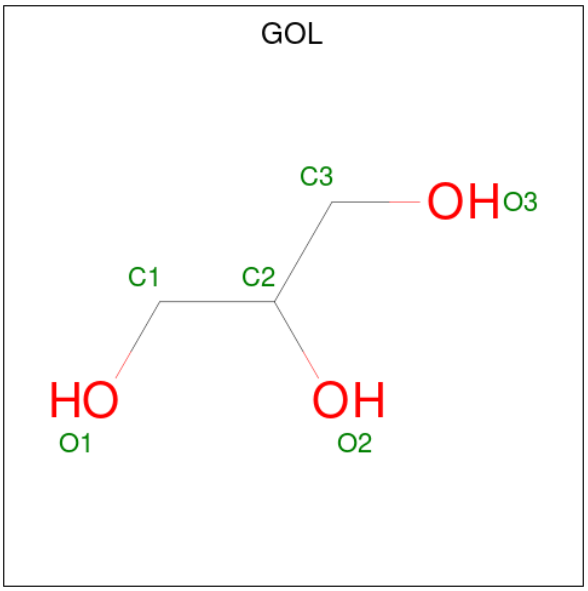
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3537	2261	615	644	17	0	38	0
1	B	435	3549	2274	614	642	19	0	41	0
1	C	436	3563	2276	620	647	20	0	42	0
1	D	436	3607	2305	632	651	19	0	47	0
1	E	435	3569	2280	623	647	19	0	43	0
1	F	436	3536	2255	622	642	17	0	37	0
1	G	436	3528	2249	619	641	19	0	34	0
1	H	436	3547	2264	622	643	18	0	39	0

- 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
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	H	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	E	1	6	3	3	0	0
			Total	C	O		
3	F	1	6	3	3	0	0
			Total	C	O		
3	G	1	6	3	3	0	0
			Total	C	O		
3	H	1	6	3	3	0	0
			Total	C	O		
3	H	1	6	3	3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
			Total	Cl		
4	B	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0
5	G	1	Total Ca 1 1	0	0
5	H	1	Total Ca 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	654	Total O 654 654	0	0
6	B	536	Total O 536 536	0	0
6	C	718	Total O 718 718	0	0
6	D	570	Total O 570 570	0	0
6	E	608	Total O 608 608	0	0
6	F	515	Total O 515 515	0	0
6	G	532	Total O 532 532	0	0

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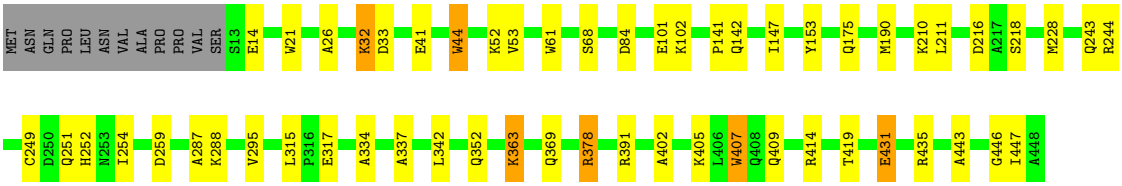
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	H	441	441	441	0	0

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.

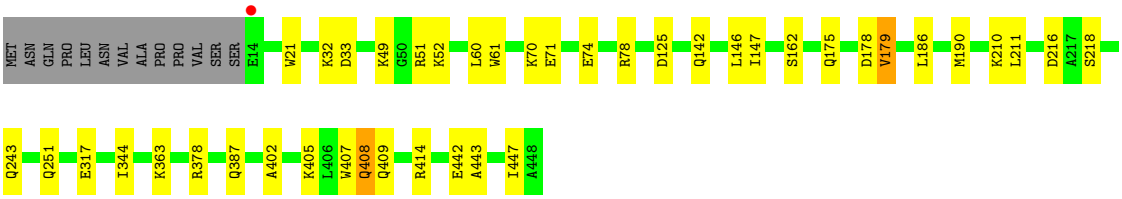
• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

Chain A:



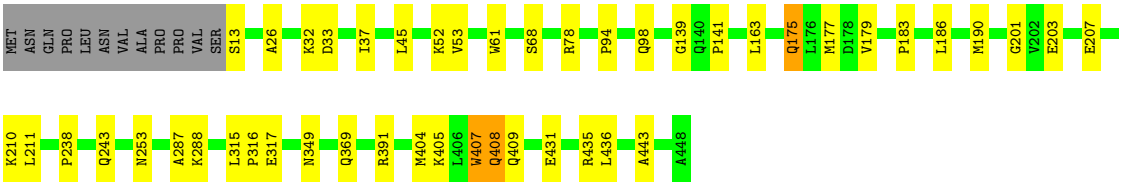
• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

Chain B:



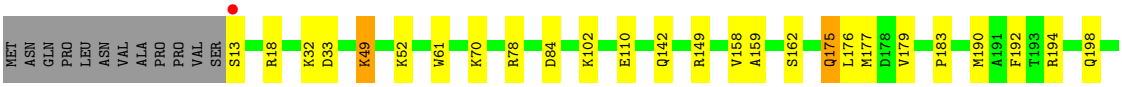
• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

Chain C:



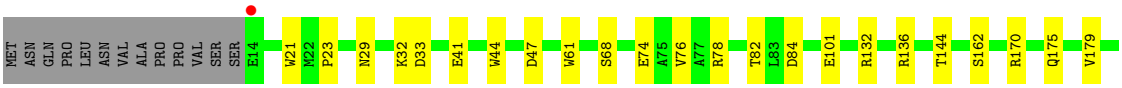
• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

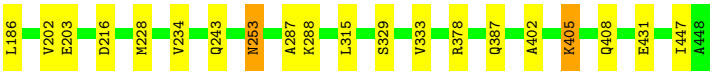
Chain D:



• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

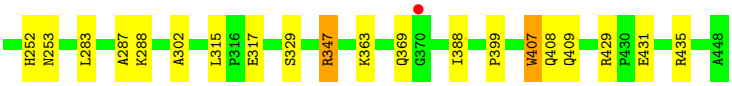
Chain E:





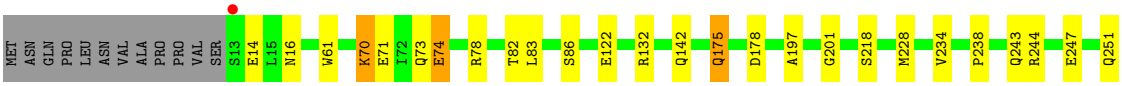
• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

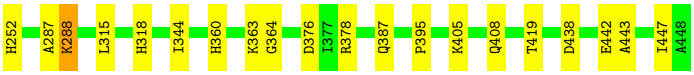
Chain F:



• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

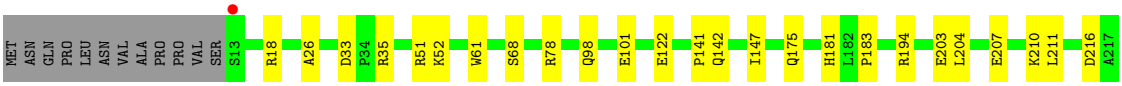
Chain G:

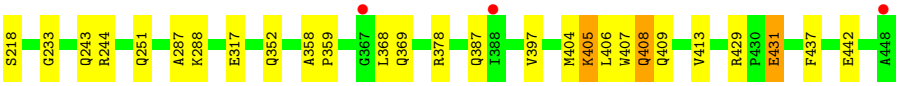




• Molecule 1: BETA-ALANINE-PYRUVATE TRANSAMINASE

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.38Å 133.16Å 161.96Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	66.58 – 1.64 66.58 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.3 (66.58-1.64) 99.3 (66.58-1.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.219 0.173 , 0.217	Depositor DCC
R_{free} test set	20738 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33210	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5891e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CL, CA, GOL, PLP

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	0.90	4/3721 (0.1%)	0.85	8/5034 (0.2%)
1	B	0.85	3/3736 (0.1%)	0.85	2/5049 (0.0%)
1	C	0.89	2/3753 (0.1%)	0.85	4/5074 (0.1%)
1	D	0.86	2/3809 (0.1%)	0.84	3/5147 (0.1%)
1	E	0.88	3/3762 (0.1%)	0.87	4/5084 (0.1%)
1	F	0.91	3/3717 (0.1%)	0.90	6/5027 (0.1%)
1	G	0.84	1/3691 (0.0%)	0.83	3/4989 (0.1%)
1	H	0.82	2/3734 (0.1%)	0.83	1/5048 (0.0%)
All	All	0.87	20/29923 (0.1%)	0.85	31/40452 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
All	All	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	407	TRP	CD2-CE2	6.56	1.49	1.41
1	C	61	TRP	CD2-CE2	6.33	1.49	1.41
1	G	61	TRP	CD2-CE2	6.14	1.48	1.41
1	F	61	TRP	CD2-CE2	5.71	1.48	1.41
1	H	61	TRP	CD2-CE2	5.69	1.48	1.41
1	A	407	TRP	CD2-CE2	5.61	1.48	1.41
1	C	407	TRP	CD2-CE2	5.42	1.47	1.41
1	F	407	TRP	CD2-CE2	5.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	61	TRP	CD2-CE2	5.29	1.47	1.41
1	A	21	TRP	CD2-CE2	5.29	1.47	1.41
1	B	61	TRP	CD2-CE2	5.29	1.47	1.41
1	H	407	TRP	CD2-CE2	5.25	1.47	1.41
1	E	21	TRP	CD2-CE2	5.18	1.47	1.41
1	B	21	TRP	CD2-CE2	5.18	1.47	1.41
1	F	44	TRP	CD2-CE2	5.18	1.47	1.41
1	A	61	TRP	CD2-CE2	5.15	1.47	1.41
1	D	407	TRP	CD2-CE2	5.08	1.47	1.41
1	E	44	TRP	CD2-CE2	5.06	1.47	1.41
1	A	44	TRP	CD2-CE2	5.03	1.47	1.41
1	D	61	TRP	CD2-CE2	5.02	1.47	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	78[A]	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	F	78[B]	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	E	84	ASP	CB-CG-OD1	7.02	124.61	118.30
1	E	228	MET	CG-SD-CE	6.96	111.34	100.20
1	A	391	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	G	315	LEU	CA-CB-CG	6.37	129.95	115.30
1	F	84	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	391	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	190	MET	CG-SD-CE	-6.12	90.41	100.20
1	A	84	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	414	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	G	228	MET	CG-SD-CE	5.92	109.67	100.20
1	F	315	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	418	ASP	CB-CG-OD1	5.74	123.46	118.30
1	C	436	LEU	CB-CG-CD2	-5.70	101.32	111.00
1	D	84	ASP	CB-CG-OD1	5.64	123.37	118.30
1	E	315	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	149	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	H	244	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	378	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	G	376	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	315	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	125	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	315	LEU	CA-CB-CG	5.21	127.30	115.30
1	F	347[A]	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	347[B]	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	47	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	244	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	414	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	177[A]	MET	CG-SD-CE	5.02	108.23	100.20
1	C	177[B]	MET	CG-SD-CE	5.02	108.23	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	THR	Peptide
1	G	419	THR	Peptide

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	3537	0	3600	55	0
1	B	3549	0	3632	55	0
1	C	3563	0	3627	59	0
1	D	3607	0	3691	56	0
1	E	3569	0	3642	41	0
1	F	3536	0	3591	45	0
1	G	3528	0	3573	44	0
1	H	3547	0	3612	51	0
2	A	16	0	7	6	0
2	B	16	0	7	1	0
2	C	16	0	7	1	0
2	D	16	0	7	3	0
2	E	16	0	7	1	0
2	F	16	0	7	1	0
2	G	16	0	7	4	0
2	H	16	0	7	1	0
3	A	12	0	16	1	0
3	B	6	0	8	3	0
3	C	12	0	16	7	0
3	E	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	6	0	8	0	0
3	G	6	0	8	1	0
3	H	12	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	654	0	0	27	0
6	B	536	0	0	37	0
6	C	718	0	0	38	0
6	D	570	0	0	29	0
6	E	608	0	0	27	0
6	F	515	0	0	20	0
6	G	532	0	0	29	0
6	H	441	0	0	26	0
All	All	33210	0	29104	411	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 7.

All (411) 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:G:70[A]:LYS:HE2	6:G:2092:HOH:O	1.23	1.35
1:H:52[A]:LYS:CE	6:H:2051:HOH:O	1.69	1.33
1:D:378[B]:ARG:NH2	1:D:387[B]:GLN:OE1	1.62	1.30
1:B:442[B]:GLU:OE2	6:B:2527:HOH:O	1.52	1.27
1:F:18[B]:ARG:NH2	6:F:2009:HOH:O	1.62	1.26
1:B:70[B]:LYS:HE2	6:B:2089:HOH:O	1.27	1.26
1:H:52[A]:LYS:HE2	6:H:2051:HOH:O	1.25	1.23
1:C:317[A]:GLU:OE2	6:C:2555:HOH:O	1.59	1.18
1:F:203[B]:GLU:OE1	6:F:2290:HOH:O	1.56	1.18
1:C:175[B]:GLN:NE2	6:C:2385:HOH:O	1.71	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:2041:HOH:O	1:F:317[A]:GLU:OE2	1.62	1.17
1:C:317[B]:GLU:OE1	6:C:2552:HOH:O	1.58	1.17
1:H:442[A]:GLU:OE1	6:H:2433:HOH:O	1.60	1.17
1:G:70[A]:LYS:CE	6:G:2092:HOH:O	1.78	1.15
1:A:175[B]:GLN:NE2	1:G:178[B]:ASP:CG	1.99	1.15
1:C:317[A]:GLU:OE1	6:C:2554:HOH:O	1.62	1.15
1:G:70[B]:LYS:NZ	6:G:2094:HOH:O	1.77	1.15
1:B:52[B]:LYS:HE2	6:B:2062:HOH:O	1.41	1.14
1:C:175[B]:GLN:CD	6:C:2385:HOH:O	1.83	1.14
1:C:175[B]:GLN:OE1	6:C:2385:HOH:O	1.63	1.14
1:A:175[B]:GLN:CD	1:G:178[B]:ASP:OD2	1.87	1.13
1:D:198[B]:GLN:NE2	6:D:2335:HOH:O	1.77	1.13
1:D:369[A]:GLN:OE1	6:D:2490:HOH:O	1.65	1.13
1:H:431[A]:GLU:OE2	6:H:2422:HOH:O	1.67	1.13
1:E:41[B]:GLU:OE2	6:E:2064:HOH:O	1.68	1.11
1:B:317[A]:GLU:OE1	6:B:2413:HOH:O	1.68	1.10
1:D:247:GLU:O	1:D:251[B]:GLN:HG2	1.55	1.07
1:H:52[A]:LYS:NZ	6:H:2051:HOH:O	1.76	1.07
6:E:2458:HOH:O	1:F:18[A]:ARG:NH1	1.69	1.06
1:E:32[B]:LYS:HD3	1:E:33[B]:ASP:OD2	1.58	1.04
1:E:32[B]:LYS:HE3	1:E:33[B]:ASP:OD2	1.57	1.04
1:E:74[B]:GLU:OE1	6:E:2130:HOH:O	1.74	1.03
1:G:318:HIS:CE1	1:H:397[B]:VAL:HG12	1.93	1.03
1:D:110[B]:GLU:HG2	6:D:2168:HOH:O	1.59	1.03
1:H:431[A]:GLU:CD	6:H:2422:HOH:O	1.97	1.02
1:H:405[B]:LYS:HE3	6:H:2411:HOH:O	1.59	1.02
1:F:18[B]:ARG:CZ	6:F:2009:HOH:O	1.89	1.02
1:A:405[B]:LYS:HG2	1:A:409[B]:GLN:HE21	1.23	1.02
1:H:405[B]:LYS:CE	6:H:2411:HOH:O	2.08	1.01
1:C:52[B]:LYS:HE3	6:C:2065:HOH:O	1.61	1.00
1:C:369[A]:GLN:O	6:C:2617:HOH:O	1.79	0.99
1:E:32[B]:LYS:CE	1:E:33[B]:ASP:OD2	2.09	0.99
1:B:52[B]:LYS:CE	6:B:2062:HOH:O	2.02	0.99
1:D:33[A]:ASP:OD2	6:D:2030:HOH:O	1.79	0.98
1:C:435[B]:ARG:NH1	6:C:2695:HOH:O	1.97	0.97
1:A:405[B]:LYS:HE2	6:A:2605:HOH:O	0.80	0.97
1:E:32[B]:LYS:CD	1:E:33[B]:ASP:OD2	2.12	0.97
1:C:98[B]:GLN:NE2	6:C:2210:HOH:O	1.79	0.96
2:D:500:PLP:O2P	6:D:2183:HOH:O	1.82	0.95
1:E:203[B]:GLU:HG3	6:E:2359:HOH:O	1.67	0.95
1:A:175[B]:GLN:HE21	1:G:178[B]:ASP:CG	1.62	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369[A]:GLN:O	6:A:2557:HOH:O	1.86	0.93
1:B:402:ALA:HB2	1:B:447[B]:ILE:HD11	1.49	0.93
6:E:2037:HOH:O	1:F:317[B]:GLU:OE1	1.87	0.92
1:B:74[B]:GLU:CD	6:B:2097:HOH:O	2.07	0.92
2:A:500:PLP:O1P	6:A:2218:HOH:O	1.88	0.91
1:A:175[B]:GLN:NE2	1:G:178[B]:ASP:OD2	0.76	0.90
1:D:49:LYS:HD2	6:D:2058:HOH:O	1.72	0.89
1:A:409[B]:GLN:NE2	6:A:2605:HOH:O	2.03	0.89
1:A:33[B]:ASP:OD2	6:A:2033:HOH:O	1.89	0.89
1:A:295[B]:VAL:HG21	1:A:334:ALA:HA	1.55	0.88
1:B:405[B]:LYS:HE2	6:B:2489:HOH:O	1.71	0.88
1:C:32[A]:LYS:NZ	6:C:2041:HOH:O	2.06	0.88
1:A:33[B]:ASP:OD2	6:A:2035:HOH:O	1.92	0.88
1:C:163:LEU:HD23	1:C:179[B]:VAL:HG11	1.56	0.88
6:D:2286:HOH:O	1:E:175[A]:GLN:HG2	1.72	0.88
1:E:203[B]:GLU:CG	6:E:2359:HOH:O	2.18	0.87
6:B:2264:HOH:O	1:G:175[A]:GLN:HG2	1.73	0.86
1:A:405[B]:LYS:HG2	1:A:409[B]:GLN:NE2	1.91	0.85
1:C:243[B]:GLN:NE2	6:C:2490:HOH:O	2.09	0.85
1:B:405[B]:LYS:HE3	1:B:443:ALA:HA	1.58	0.85
1:E:203[B]:GLU:OE2	6:E:2359:HOH:O	1.93	0.84
1:E:29:ASN:OD1	6:E:2028:HOH:O	1.94	0.84
1:E:74[A]:GLU:OE1	6:E:2130:HOH:O	1.94	0.84
2:C:500:PLP:O1P	6:C:2245:HOH:O	1.96	0.84
1:D:198[B]:GLN:CD	1:D:198[B]:GLN:H	1.83	0.82
1:D:175[A]:GLN:HG2	6:D:2288:HOH:O	1.79	0.82
1:B:363[B]:LYS:HE2	6:B:2448:HOH:O	1.78	0.81
3:E:504:GOL:H2	6:E:2608:HOH:O	1.79	0.81
2:H:500:PLP:O1P	6:H:2141:HOH:O	1.97	0.81
3:C:504:GOL:H2	6:C:2715:HOH:O	1.80	0.81
2:A:500:PLP:H2A1	6:A:2462:HOH:O	1.81	0.81
1:B:186[B]:LEU:HD12	6:B:2092:HOH:O	1.80	0.81
1:C:211[B]:LEU:HD11	3:C:504:GOL:H31	1.63	0.80
1:G:70[A]:LYS:NZ	6:G:2092:HOH:O	1.97	0.80
1:G:74[A]:GLU:HG3	6:G:2032:HOH:O	1.80	0.80
1:D:18[A]:ARG:NH1	6:D:2012:HOH:O	2.14	0.80
1:B:251[A]:GLN:OE1	6:B:2368:HOH:O	1.98	0.80
1:H:405[B]:LYS:HD2	6:H:2411:HOH:O	1.81	0.80
1:B:363[B]:LYS:CE	6:B:2448:HOH:O	2.30	0.80
2:F:500:PLP:O3P	6:F:2158:HOH:O	1.99	0.80
1:H:405[B]:LYS:NZ	6:H:2410:HOH:O	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211[B]:LEU:CD1	3:C:504:GOL:H31	2.12	0.78
2:E:500:PLP:O1P	6:E:2217:HOH:O	2.02	0.78
1:B:190[B]:MET:HE1	6:B:2288:HOH:O	1.83	0.78
1:E:132[B]:ARG:HH21	1:F:174:GLY:HA3	1.49	0.78
3:A:504:GOL:H32	6:A:2654:HOH:O	1.83	0.77
1:F:369[B]:GLN:O	6:F:2435:HOH:O	2.01	0.77
1:C:431[A]:GLU:HG3	6:C:2686:HOH:O	1.83	0.77
1:B:74[B]:GLU:OE2	6:B:2097:HOH:O	1.99	0.76
1:H:369[B]:GLN:O	6:H:2384:HOH:O	2.03	0.76
1:D:194[B]:ARG:HD3	6:D:2323:HOH:O	1.83	0.76
1:C:163:LEU:HD23	1:C:179[B]:VAL:CG1	2.17	0.75
1:D:52[B]:LYS:HE2	6:D:2051:HOH:O	1.86	0.75
1:E:405[B]:LYS:HE3	1:E:405[B]:LYS:HA	1.68	0.75
1:G:243[A]:GLN:HG3	6:G:2336:HOH:O	1.86	0.74
1:A:431[A]:GLU:CG	1:A:435:ARG:HH22	2.00	0.74
1:D:110[B]:GLU:OE2	6:D:2173:HOH:O	2.05	0.74
1:C:405[B]:LYS:HD2	1:C:443:ALA:HA	1.67	0.74
1:G:363[B]:LYS:HE3	6:G:2446:HOH:O	1.88	0.73
1:A:102[B]:LYS:NZ	1:A:342:LEU:HB3	2.04	0.73
1:D:243[A]:GLN:OE1	6:D:2387:HOH:O	2.05	0.73
2:B:500:PLP:O1P	6:B:2164:HOH:O	2.06	0.72
1:C:203[A]:GLU:HG2	6:C:2444:HOH:O	1.87	0.72
1:G:408[A]:GLN:HG2	6:G:2491:HOH:O	1.88	0.72
2:G:500:PLP:O1P	6:G:2172:HOH:O	2.06	0.72
1:A:431[A]:GLU:HG2	1:A:435:ARG:NH2	2.06	0.70
3:C:504:GOL:H32	6:C:2453:HOH:O	1.91	0.70
1:D:78[B]:ARG:HG3	1:D:78[B]:ARG:HH11	1.55	0.70
1:H:243[B]:GLN:OE1	6:H:2274:HOH:O	0.70	0.70
1:H:78[A]:ARG:HD2	6:H:2091:HOH:O	1.92	0.69
1:A:317[A]:GLU:H	1:A:317[A]:GLU:CD	1.93	0.69
6:C:2392:HOH:O	1:E:175[B]:GLN:NE2	2.24	0.69
1:D:18[B]:ARG:NH1	6:D:2010:HOH:O	2.25	0.69
1:G:247:GLU:OE1	6:G:2342:HOH:O	2.09	0.69
1:A:102[B]:LYS:HZ1	1:A:342:LEU:HB3	1.57	0.68
1:B:405[B]:LYS:HD2	1:B:443:ALA:CB	2.23	0.68
1:C:431[B]:GLU:CD	1:C:431[B]:GLU:H	1.97	0.68
1:E:74[B]:GLU:OE1	6:E:2131:HOH:O	2.10	0.68
3:G:504:GOL:H32	6:G:2532:HOH:O	1.94	0.68
1:H:181:HIS:O	3:H:504:GOL:O1	2.12	0.68
1:D:198[B]:GLN:CD	6:D:2335:HOH:O	2.18	0.67
1:D:369[B]:GLN:NE2	6:D:2327:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295[B]:VAL:CG2	1:A:334:ALA:HA	2.23	0.67
6:G:2164:HOH:O	1:H:18[A]:ARG:NH2	2.27	0.67
1:C:404:MET:O	1:C:408[B]:GLN:HG2	1.93	0.67
1:A:101:GLU:HG3	6:A:2184:HOH:O	1.94	0.67
1:F:363[B]:LYS:HD2	6:F:2088:HOH:O	1.93	0.67
1:B:363[B]:LYS:HE2	6:B:2441:HOH:O	1.94	0.66
1:C:78[B]:ARG:NH2	6:C:2150:HOH:O	1.81	0.66
1:G:318:HIS:CE1	1:H:397[B]:VAL:CG1	2.76	0.66
1:C:210[B]:LYS:HE3	6:C:2458:HOH:O	1.94	0.66
1:A:153:TYR:O	2:A:500:PLP:H2A3	1.96	0.66
1:D:378[A]:ARG:HD2	6:D:2382:HOH:O	1.95	0.66
1:F:347[A]:ARG:NH2	6:F:2397:HOH:O	2.28	0.65
1:H:431[A]:GLU:OE1	6:H:2422:HOH:O	2.07	0.65
1:B:70[B]:LYS:CE	6:B:2088:HOH:O	2.45	0.65
1:F:175[B]:GLN:HG2	6:F:2247:HOH:O	1.96	0.65
1:E:378[A]:ARG:HD2	6:E:2390:HOH:O	1.95	0.65
1:G:443:ALA:O	1:G:447[B]:ILE:HD12	1.96	0.64
1:F:408[B]:GLN:HG2	6:F:2470:HOH:O	1.96	0.64
1:C:211[B]:LEU:CD1	3:C:504:GOL:C3	2.76	0.64
1:B:378[B]:ARG:NH2	1:B:387:GLN:OE1	2.31	0.64
1:B:70[B]:LYS:HE3	6:B:2088:HOH:O	1.97	0.64
1:C:186[A]:LEU:HD13	6:C:2134:HOH:O	1.98	0.63
1:A:405[B]:LYS:HD3	1:A:443:ALA:HA	1.81	0.63
1:B:402:ALA:HB2	1:B:447[B]:ILE:CD1	2.27	0.63
1:C:405[B]:LYS:CE	6:C:2662:HOH:O	2.46	0.63
1:F:435[B]:ARG:HD3	6:F:2500:HOH:O	1.96	0.63
1:G:288:LYS:CE	2:G:500:PLP:O4A	2.47	0.63
1:G:442[B]:GLU:HG2	6:G:2492:HOH:O	1.97	0.63
1:E:74[B]:GLU:CD	6:E:2130:HOH:O	2.26	0.62
1:G:70[B]:LYS:HE3	1:G:73:GLN:OE1	1.98	0.62
1:D:408[A]:GLN:NE2	1:D:409:GLN:OE1	2.33	0.62
1:H:78[A]:ARG:NH1	6:H:2091:HOH:O	2.32	0.61
1:D:70[A]:LYS:HE2	6:D:2084:HOH:O	1.99	0.61
1:D:192:PHE:CD1	1:D:369[B]:GLN:HG3	2.36	0.61
6:A:2334:HOH:O	1:G:132:ARG:NH2	2.28	0.61
1:A:210[A]:LYS:HE3	6:A:2404:HOH:O	2.00	0.60
1:C:211[A]:LEU:HD21	3:C:504:GOL:H31	1.84	0.60
1:D:190:MET:CE	1:D:198[B]:GLN:HE22	2.15	0.60
1:C:349[B]:ASN:HB2	6:C:2582:HOH:O	2.01	0.60
1:F:102[A]:LYS:HE2	6:F:2133:HOH:O	2.01	0.60
1:C:203[A]:GLU:CG	6:C:2444:HOH:O	2.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:429[A]:ARG:NE	6:H:2422:HOH:O	2.35	0.60
1:E:186[B]:LEU:HD12	6:E:2122:HOH:O	2.01	0.59
1:G:378[B]:ARG:NH2	1:G:387:GLN:OE1	2.35	0.59
1:A:243[A]:GLN:HG3	6:A:2434:HOH:O	2.03	0.59
1:A:251[A]:GLN:HG3	6:A:2450:HOH:O	2.02	0.59
1:D:192:PHE:HB3	1:D:369[B]:GLN:HE21	1.68	0.58
1:B:243[B]:GLN:CG	6:B:2354:HOH:O	2.51	0.58
1:G:16[B]:ASN:ND2	6:G:2002:HOH:O	2.36	0.58
1:E:408[B]:GLN:HG2	6:E:2556:HOH:O	2.04	0.58
1:H:183:PRO:HG3	1:H:207:GLU:HG3	1.86	0.58
1:E:203[B]:GLU:CD	6:E:2359:HOH:O	2.32	0.58
1:F:317[B]:GLU:OE1	6:F:2384:HOH:O	2.17	0.58
1:H:368:LEU:HD21	1:H:437:PHE:HB3	1.86	0.58
1:D:431[B]:GLU:HG2	6:D:2552:HOH:O	2.03	0.57
1:G:252:HIS:HD2	6:G:2354:HOH:O	1.87	0.57
1:B:33:ASP:OD2	6:B:2025:HOH:O	2.18	0.57
1:F:408[B]:GLN:NE2	1:F:409:GLN:OE1	2.37	0.57
1:H:210[B]:LYS:HE3	6:H:2258:HOH:O	2.04	0.57
1:A:175[B]:GLN:OE1	1:A:175[B]:GLN:HA	2.04	0.57
1:D:402:ALA:HB2	1:D:447[A]:ILE:HD11	1.85	0.57
1:F:140[B]:GLN:NE2	6:F:2192:HOH:O	2.36	0.57
1:A:352[B]:GLN:HG3	6:A:2533:HOH:O	2.04	0.57
1:B:147[B]:ILE:HD13	1:B:211[B]:LEU:HD23	1.84	0.57
1:H:352[A]:GLN:NE2	6:H:2358:HOH:O	0.72	0.57
1:E:243[A]:GLN:HG3	6:E:2395:HOH:O	2.03	0.57
1:H:35:ARG:NH1	1:H:404[B]:MET:HE3	2.19	0.57
1:C:203[A]:GLU:CD	6:C:2444:HOH:O	2.44	0.57
1:D:70[A]:LYS:HG2	6:D:2084:HOH:O	2.03	0.56
1:F:78[A]:ARG:NH1	6:F:2092:HOH:O	2.37	0.56
1:C:391[B]:ARG:HD2	6:C:2644:HOH:O	2.04	0.56
1:D:190:MET:HE1	1:D:198[B]:GLN:HE22	1.69	0.56
1:H:147[B]:ILE:HD12	1:H:211[B]:LEU:HD23	1.87	0.56
1:H:405[B]:LYS:CD	6:H:2411:HOH:O	2.32	0.56
1:C:408[A]:GLN:OE1	1:C:409:GLN:NE2	2.30	0.56
6:E:2041:HOH:O	1:F:317[A]:GLU:CD	2.24	0.56
3:E:504:GOL:H11	6:E:2367:HOH:O	2.06	0.55
1:A:405[A]:LYS:HZ1	1:A:446:GLY:HA3	1.70	0.55
2:A:500:PLP:C2A	6:A:2462:HOH:O	2.48	0.55
1:D:369[A]:GLN:HG3	1:D:370:GLY:N	2.22	0.55
1:A:141:PRO:HG2	1:H:141:PRO:HG2	1.89	0.55
3:B:504:GOL:H32	6:B:2536:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405[B]:LYS:HE3	6:C:2662:HOH:O	2.06	0.55
1:B:178[B]:ASP:OD2	1:H:175[B]:GLN:NE2	2.40	0.54
1:F:210[A]:LYS:HE3	6:F:2300:HOH:O	2.07	0.54
1:A:431[A]:GLU:CG	1:A:435:ARG:NH2	2.66	0.54
1:E:74[B]:GLU:CG	6:E:2130:HOH:O	2.55	0.54
1:G:16[B]:ASN:H	1:G:16[B]:ASN:HD22	1.54	0.54
1:H:35:ARG:NH1	1:H:404[B]:MET:CE	2.70	0.54
1:B:74[B]:GLU:OE1	6:B:2097:HOH:O	2.17	0.54
1:A:431[B]:GLU:CD	1:A:435:ARG:HH12	2.11	0.54
1:C:94:PRO:O	1:C:98[B]:GLN:HG3	2.08	0.54
1:G:16[B]:ASN:HD21	1:H:101:GLU:HB2	1.73	0.53
1:B:405[B]:LYS:HD2	1:B:443:ALA:HB1	1.90	0.53
1:A:14:GLU:HB2	6:A:2002:HOH:O	2.08	0.53
1:A:44:TRP:CE3	1:A:52[B]:LYS:HG2	2.43	0.53
1:F:71:GLU:HG2	1:F:347[B]:ARG:HH21	1.74	0.53
6:G:2400:HOH:O	1:H:26:ALA:HB1	2.09	0.53
1:B:210[B]:LYS:HE3	6:B:2327:HOH:O	2.09	0.53
1:A:431[A]:GLU:HG3	1:A:435:ARG:HH22	1.73	0.52
1:C:317[A]:GLU:CD	6:C:2555:HOH:O	2.25	0.52
6:C:2555:HOH:O	1:D:32[A]:LYS:NZ	2.08	0.52
1:E:431[A]:GLU:HG3	6:E:2300:HOH:O	2.08	0.52
1:G:360:HIS:O	6:G:2435:HOH:O	2.19	0.52
1:B:32[B]:LYS:HE2	6:B:2024:HOH:O	2.09	0.52
1:C:405[B]:LYS:HD2	1:C:443:ALA:CA	2.37	0.52
6:D:2365:HOH:O	1:F:170[B]:ARG:HG3	2.09	0.52
1:E:378[B]:ARG:NH2	1:E:387:GLN:OE1	2.43	0.52
1:B:405[B]:LYS:CE	1:B:443:ALA:HA	2.33	0.51
1:G:142[B]:GLN:HG2	1:G:218:SER:O	2.09	0.51
1:A:41[A]:GLU:HG2	6:A:2053:HOH:O	2.09	0.51
1:B:405[B]:LYS:CE	6:B:2489:HOH:O	2.42	0.51
1:A:402:ALA:HB2	1:A:447[A]:ILE:CD1	2.40	0.51
1:A:259:ASP:OD1	2:A:500:PLP:H2A2	2.11	0.51
1:A:378:ARG:HD2	6:A:2429:HOH:O	2.11	0.51
1:F:363[B]:LYS:NZ	1:F:363[B]:LYS:HB3	2.25	0.51
1:A:32[B]:LYS:NZ	1:B:317[B]:GLU:OE2	2.36	0.51
2:G:500:PLP:H4A	6:G:2531:HOH:O	2.11	0.51
1:A:147[B]:ILE:HD12	1:A:211[B]:LEU:HD23	1.93	0.50
1:A:405[A]:LYS:NZ	1:A:446:GLY:HA3	2.26	0.50
1:C:52[B]:LYS:HB3	1:C:52[B]:LYS:HZ3	1.76	0.50
1:C:211[B]:LEU:HD11	3:C:504:GOL:C3	2.39	0.50
1:G:363[B]:LYS:HG3	6:G:2434:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52[B]:LYS:HE3	6:B:2062:HOH:O	1.88	0.50
1:D:247:GLU:O	1:D:251[B]:GLN:CG	2.43	0.50
1:G:405[B]:LYS:HE3	6:G:2494:HOH:O	2.11	0.50
1:A:363[A]:LYS:HB3	1:A:363[A]:LYS:NZ	2.27	0.50
1:C:78[B]:ARG:NE	6:C:2150:HOH:O	2.44	0.50
1:A:431[B]:GLU:OE2	6:A:2627:HOH:O	0.50	0.49
1:B:49[B]:LYS:HG2	6:B:2055:HOH:O	2.11	0.49
1:E:68[B]:SER:HB2	6:E:2059:HOH:O	2.12	0.49
1:B:243[B]:GLN:CD	6:B:2354:HOH:O	2.50	0.49
1:B:408[A]:GLN:NE2	1:B:409:GLN:OE1	2.45	0.49
1:G:364:GLY:HA3	6:G:2435:HOH:O	2.12	0.49
1:H:406:LEU:HD13	1:H:413:VAL:HG21	1.93	0.49
1:D:192:PHE:HB3	1:D:369[B]:GLN:NE2	2.27	0.49
1:C:405[B]:LYS:CD	1:C:443:ALA:HA	2.39	0.49
1:E:243[B]:GLN:NE2	6:E:2399:HOH:O	2.46	0.48
1:H:405[A]:LYS:NZ	1:H:408[A]:GLN:HE22	2.11	0.48
1:G:201:GLY:HA2	1:G:238:PRO:HG2	1.95	0.48
1:H:142[B]:GLN:HG2	1:H:218:SER:O	2.13	0.48
6:A:2564:HOH:O	1:D:18[A]:ARG:NH2	2.47	0.48
1:B:363[B]:LYS:HE3	6:B:2448:HOH:O	2.04	0.48
1:G:288:LYS:HE2	2:G:500:PLP:O4A	2.12	0.48
1:C:175[B]:GLN:NE2	1:E:144:THR:OG1	2.47	0.48
1:H:78[A]:ARG:NH2	6:H:2090:HOH:O	2.47	0.48
1:C:33[B]:ASP:OD1	6:C:2039:HOH:O	2.20	0.47
1:H:203[B]:GLU:HG2	1:H:204:LEU:N	2.30	0.47
1:B:142[B]:GLN:HG2	1:B:218:SER:O	2.14	0.47
6:C:2566:HOH:O	2:D:500:PLP:O3P	0.63	0.47
6:G:2119:HOH:O	1:H:68[B]:SER:HB2	2.15	0.47
6:E:2041:HOH:O	1:F:317[A]:GLU:CG	2.60	0.47
1:B:402:ALA:CB	1:B:447[B]:ILE:HD11	2.34	0.47
1:D:194[B]:ARG:CD	6:D:2323:HOH:O	2.54	0.47
1:E:162:SER:O	1:E:179[B]:VAL:HG21	2.15	0.47
1:F:201:GLY:HA2	1:F:238:PRO:HG2	1.96	0.47
1:D:78[B]:ARG:HG3	1:D:78[B]:ARG:NH1	2.28	0.47
1:F:429[B]:ARG:NH1	1:F:431[B]:GLU:OE1	2.46	0.47
1:A:363[B]:LYS:HE2	6:A:2237:HOH:O	2.14	0.47
1:B:175[A]:GLN:NE2	6:B:2266:HOH:O	2.27	0.47
1:B:186[A]:LEU:HD22	6:B:2286:HOH:O	2.13	0.47
1:C:175[A]:GLN:HG2	1:F:175[A]:GLN:HG2	1.97	0.46
1:F:363[B]:LYS:CD	6:F:2088:HOH:O	2.58	0.46
6:G:2130:HOH:O	1:H:35:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:ARG:NH1	6:H:2234:HOH:O	2.44	0.46
6:D:2374:HOH:O	1:E:136:ARG:NH1	2.45	0.46
1:C:139:GLY:C	1:C:141:PRO:HD3	2.36	0.46
1:G:78[B]:ARG:HH21	1:G:82:THR:CB	2.29	0.46
1:F:53:VAL:HG11	1:F:407:TRP:CZ3	2.50	0.46
1:D:401:GLU:HB3	1:D:447[B]:ILE:HD12	1.98	0.46
1:C:53:VAL:HG11	1:C:407:TRP:CZ3	2.51	0.46
1:D:283:LEU:HD23	1:D:302:ALA:HA	1.97	0.46
1:A:243[B]:GLN:NE2	6:A:2439:HOH:O	2.47	0.46
1:G:122:GLU:OE2	1:H:122:GLU:HG3	2.16	0.46
1:A:402:ALA:HB2	1:A:447[A]:ILE:HD11	1.97	0.45
1:D:78[A]:ARG:HD3	6:D:2103:HOH:O	2.16	0.45
1:F:317[B]:GLU:CD	6:F:2384:HOH:O	2.53	0.45
1:G:252:HIS:CD2	6:G:2354:HOH:O	2.66	0.45
1:B:378[A]:ARG:HD2	6:B:2349:HOH:O	2.16	0.45
1:G:244:ARG:NH1	6:G:2342:HOH:O	2.49	0.45
1:G:438:ASP:HB3	6:G:2524:HOH:O	2.16	0.45
6:C:2566:HOH:O	2:D:500:PLP:P	1.15	0.45
1:C:183:PRO:HG3	1:C:207:GLU:HG3	1.99	0.45
1:C:316:PRO:HG2	6:D:2520:HOH:O	2.15	0.45
1:D:159:ALA:HA	1:D:177[B]:MET:SD	2.57	0.45
1:C:243[B]:GLN:CG	6:C:2490:HOH:O	2.64	0.44
1:F:252:HIS:HD2	6:F:2340:HOH:O	2.00	0.44
1:E:76:VAL:HG13	1:E:333:VAL:HG13	2.00	0.44
1:F:253[B]:ASN:HD22	1:F:253[B]:ASN:HA	1.63	0.44
1:D:402:ALA:HB2	1:D:447[A]:ILE:CD1	2.47	0.44
3:B:504:GOL:H11	6:B:2536:HOH:O	2.18	0.44
1:C:405[B]:LYS:HE3	1:C:405[B]:LYS:HB2	1.69	0.44
1:D:142[B]:GLN:HG2	1:D:218:SER:O	2.17	0.44
1:E:23:PRO:HG3	1:F:329:SER:HB2	2.00	0.44
1:G:78[A]:ARG:HG3	6:G:2103:HOH:O	2.18	0.44
1:H:429[A]:ARG:NH2	6:H:2422:HOH:O	2.50	0.44
1:G:71:GLU:HB2	1:G:344:ILE:HD11	1.99	0.44
1:C:175[A]:GLN:HG2	1:F:175[A]:GLN:CD	2.39	0.43
1:D:258:PHE:HB2	1:D:281:PRO:HG3	2.01	0.43
1:C:201:GLY:HA2	1:C:238:PRO:HG2	2.01	0.43
1:D:431[B]:GLU:CG	6:D:2552:HOH:O	2.64	0.43
1:A:26:ALA:HB1	6:A:2028:HOH:O	2.18	0.43
1:D:251[B]:GLN:HG2	1:D:251[B]:GLN:H	1.65	0.43
1:H:405[A]:LYS:HE2	1:H:409:GLN:HG2	2.01	0.43
1:C:163:LEU:CD2	1:C:179[B]:VAL:CG1	2.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:SER:HB2	6:A:2047:HOH:O	2.19	0.43
1:F:363[B]:LYS:NZ	1:F:363[B]:LYS:CB	2.81	0.43
1:B:49[A]:LYS:HG3	1:B:51:ARG:HG3	2.01	0.43
1:B:210[B]:LYS:NZ	6:B:2315:HOH:O	2.51	0.43
1:D:158:VAL:HG13	1:D:176[A]:LEU:HB3	2.01	0.43
1:A:295[B]:VAL:HG22	1:A:337:ALA:HB3	2.00	0.43
1:A:102[B]:LYS:NZ	1:A:342:LEU:CB	2.78	0.42
1:D:162:SER:O	1:D:179[B]:VAL:HG21	2.19	0.42
1:D:253[A]:ASN:HD22	1:D:253[A]:ASN:HA	1.69	0.42
1:H:98:GLN:NE2	6:H:2119:HOH:O	2.53	0.42
1:E:78[B]:ARG:HH22	1:E:82:THR:HG21	1.85	0.42
1:B:405[A]:LYS:HA	1:B:408[A]:GLN:HG2	2.01	0.42
1:D:175[A]:GLN:NE2	6:D:2289:HOH:O	2.51	0.42
1:A:142[B]:GLN:HG2	1:A:218:SER:O	2.20	0.42
1:B:71:GLU:HB2	1:B:344:ILE:HD11	2.01	0.42
1:E:170[A]:ARG:NH2	6:E:2316:HOH:O	2.52	0.42
1:A:53:VAL:HG11	1:A:407:TRP:CZ3	2.54	0.42
1:B:405[B]:LYS:HE3	1:B:443:ALA:CA	2.40	0.42
1:E:329:SER:HB2	1:F:23:PRO:HG3	2.02	0.42
1:E:402:ALA:HB2	1:E:447[B]:ILE:CD1	2.50	0.42
1:F:140[B]:GLN:NE2	1:F:142[B]:GLN:HE22	2.17	0.42
1:H:378[B]:ARG:NH2	1:H:387:GLN:OE1	2.52	0.42
1:F:142[B]:GLN:HG2	1:F:218:SER:O	2.19	0.42
1:F:388[A]:ILE:HD12	1:F:399:PRO:HG3	2.02	0.42
1:C:37:ILE:HD13	1:C:45:LEU:HD13	2.01	0.42
1:C:190[B]:MET:HE2	1:C:190[B]:MET:HB3	1.84	0.41
6:C:2010:HOH:O	1:D:308:ASP:OD1	2.22	0.41
1:G:197:ALA:HB3	1:G:238:PRO:HB3	2.01	0.41
1:C:68:SER:HB2	6:C:2060:HOH:O	2.19	0.41
1:C:317[A]:GLU:CG	6:C:2555:HOH:O	2.67	0.41
1:B:408[A]:GLN:HG3	1:B:409:GLN:N	2.36	0.41
1:C:52[B]:LYS:HB3	1:C:52[B]:LYS:NZ	2.35	0.41
1:D:110[B]:GLU:HG2	1:D:110[B]:GLU:H	1.61	0.41
1:D:210[A]:LYS:HE2	6:D:2358:HOH:O	2.20	0.41
1:G:83:LEU:HD11	1:G:86[A]:SER:HB3	2.03	0.41
1:C:26:ALA:HB1	6:C:2023:HOH:O	2.19	0.41
1:H:251[A]:GLN:NE2	6:H:2282:HOH:O	2.36	0.41
1:B:60[B]:LEU:HD23	1:B:60[B]:LEU:HA	1.77	0.41
1:B:190[B]:MET:CE	6:B:2288:HOH:O	2.54	0.41
6:D:2236:HOH:O	1:F:175[A]:GLN:HG3	2.20	0.41
1:F:283:LEU:HD23	1:F:302:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:405[A]:LYS:NZ	1:H:408[A]:GLN:NE2	2.69	0.41
1:B:146:LEU:HB2	1:B:179[A]:VAL:HG12	2.02	0.41
3:B:504:GOL:C3	6:B:2536:HOH:O	2.67	0.41
1:B:162:SER:O	1:B:179[B]:VAL:HG21	2.20	0.41
1:D:237:PRO:HA	1:D:238:PRO:HD3	2.00	0.41
1:E:101[B]:GLU:OE1	1:F:16:ASN:ND2	2.54	0.41
1:E:431[A]:GLU:H	1:E:431[A]:GLU:CD	2.24	0.41
1:F:32[B]:LYS:HB3	1:F:32[B]:LYS:HE2	1.92	0.41
1:G:251[B]:GLN:HG3	6:G:2352:HOH:O	2.20	0.41
1:A:363[A]:LYS:NZ	6:A:2551:HOH:O	2.48	0.41
1:B:32[A]:LYS:HE3	6:B:2017:HOH:O	2.21	0.41
1:D:183:PRO:HG3	1:D:207:GLU:HG3	2.02	0.41
1:E:253[A]:ASN:HD22	1:E:253[A]:ASN:HA	1.73	0.41
1:F:435[B]:ARG:NH1	6:F:2496:HOH:O	2.54	0.41
1:F:211[B]:LEU:CD1	6:F:2295:HOH:O	2.67	0.40
1:G:74[B]:GLU:HG2	6:G:2104:HOH:O	2.21	0.40
1:A:102[B]:LYS:HZ2	1:A:342:LEU:HB3	1.84	0.40
1:A:249:CYS:HB3	1:A:254:ILE:O	2.21	0.40
2:A:500:PLP:O2P	6:A:2221:HOH:O	1.69	0.40
1:H:210[B]:LYS:HE2	6:H:2255:HOH:O	2.22	0.40
1:H:358:ALA:HB3	1:H:359:PRO:HD3	2.03	0.40
1:A:252:HIS:HD2	6:A:2457:HOH:O	2.03	0.40
1:D:102:LYS:HB2	1:D:102:LYS:HE2	1.87	0.40
1:H:233:GLY:O	1:H:378[B]:ARG:NH1	2.50	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	472/448 (105%)	453 (96%)	16 (3%)	3 (1%)	25 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/448 (106%)	458 (97%)	15 (3%)	1 (0%)	47	26
1	C	476/448 (106%)	459 (96%)	15 (3%)	2 (0%)	34	15
1	D	481/448 (107%)	466 (97%)	11 (2%)	4 (1%)	19	4
1	E	476/448 (106%)	462 (97%)	10 (2%)	4 (1%)	19	4
1	F	471/448 (105%)	454 (96%)	14 (3%)	3 (1%)	25	8
1	G	468/448 (104%)	448 (96%)	17 (4%)	3 (1%)	25	8
1	H	473/448 (106%)	456 (96%)	14 (3%)	3 (1%)	25	8
All	All	3791/3584 (106%)	3656 (96%)	112 (3%)	23 (1%)	22	8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	C	288	LYS
1	D	288	LYS
1	G	288	LYS
1	H	288	LYS
1	D	287	ALA
1	F	287	ALA
1	F	288	LYS
1	H	287	ALA
1	A	216	ASP
1	A	287	ALA
1	B	216	ASP
1	E	216	ASP
1	E	287	ALA
1	E	288	LYS
1	G	287	ALA
1	H	216	ASP
1	C	287	ALA
1	D	216	ASP
1	F	216	ASP
1	D	234	VAL
1	G	234	VAL
1	E	234	VAL

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	376/350 (107%)	369 (98%)	7 (2%)	57	32
1	B	379/350 (108%)	375 (99%)	4 (1%)	73	55
1	C	380/350 (109%)	373 (98%)	7 (2%)	59	34
1	D	386/350 (110%)	378 (98%)	8 (2%)	53	26
1	E	381/350 (109%)	377 (99%)	4 (1%)	76	59
1	F	375/350 (107%)	371 (99%)	4 (1%)	73	55
1	G	373/350 (107%)	365 (98%)	8 (2%)	53	26
1	H	377/350 (108%)	368 (98%)	9 (2%)	49	21
All	All	3027/2800 (108%)	2976 (98%)	51 (2%)	73	36

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

Mol	Chain	Res	Type
1	A	32[A]	LYS
1	A	32[B]	LYS
1	A	228	MET
1	A	363[A]	LYS
1	A	363[B]	LYS
1	A	431[A]	GLU
1	A	431[B]	GLU
1	B	179[A]	VAL
1	B	179[B]	VAL
1	B	408[A]	GLN
1	B	408[B]	GLN
1	C	13	SER
1	C	175[A]	GLN
1	C	175[B]	GLN
1	C	253[A]	ASN
1	C	253[B]	ASN
1	C	408[A]	GLN
1	C	408[B]	GLN
1	D	13	SER

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Mol	Chain	Res	Type
1	D	49	LYS
1	D	175[A]	GLN
1	D	175[B]	GLN
1	D	228[A]	MET
1	D	228[B]	MET
1	D	253[A]	ASN
1	D	253[B]	ASN
1	E	253[A]	ASN
1	E	253[B]	ASN
1	E	405[A]	LYS
1	E	405[B]	LYS
1	F	14	GLU
1	F	49	LYS
1	F	175[A]	GLN
1	F	175[B]	GLN
1	G	14	GLU
1	G	70[A]	LYS
1	G	70[B]	LYS
1	G	74[A]	GLU
1	G	74[B]	GLU
1	G	175[A]	GLN
1	G	175[B]	GLN
1	G	395	PRO
1	H	51	ARG
1	H	317[A]	GLU
1	H	317[B]	GLU
1	H	405[A]	LYS
1	H	405[B]	LYS
1	H	408[A]	GLN
1	H	408[B]	GLN
1	H	431[A]	GLU
1	H	431[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	169	ASN
1	B	312	ASN
1	B	409	GLN
1	C	373	ASN
1	D	169	ASN

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Mol	Chain	Res	Type
1	D	409	GLN
1	E	169	ASN
1	F	79	GLN
1	F	373	ASN
1	F	409	GLN
1	G	187	GLN
1	G	252	HIS
1	G	373	ASN
1	G	409	GLN
1	H	98	GLN
1	H	252	HIS
1	H	349	ASN
1	H	373	ASN
1	H	409	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)

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 for Mogul analysis.

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	PLP	F	500	-	16,16,16	2.74	5 (31%)	20,23,23	2.46	10 (50%)
3	GOL	B	504	-	5,5,5	0.41	0	5,5,5	1.34	1 (20%)
3	GOL	F	501	-	5,5,5	0.65	0	5,5,5	0.68	0
3	GOL	H	504	-	5,5,5	0.28	0	5,5,5	0.45	0
3	GOL	E	504	-	5,5,5	0.48	0	5,5,5	0.62	0
2	PLP	A	500	-	16,16,16	3.40	4 (25%)	20,23,23	2.26	9 (45%)
3	GOL	G	504	-	5,5,5	0.43	0	5,5,5	1.29	0
3	GOL	A	504	-	5,5,5	0.30	0	5,5,5	1.12	0
2	PLP	G	500	-	16,16,16	2.94	5 (31%)	20,23,23	2.24	7 (35%)
3	GOL	C	501	-	5,5,5	0.38	0	5,5,5	1.06	1 (20%)
2	PLP	D	500	-	16,16,16	2.70	6 (37%)	20,23,23	2.16	9 (45%)
3	GOL	A	501	-	5,5,5	0.58	0	5,5,5	0.39	0
2	PLP	C	500	-	16,16,16	3.06	6 (37%)	20,23,23	2.43	8 (40%)
2	PLP	H	500	-	16,16,16	2.95	4 (25%)	20,23,23	1.66	6 (30%)
3	GOL	C	504	-	5,5,5	0.31	0	5,5,5	1.07	0
2	PLP	B	500	-	16,16,16	2.85	7 (43%)	20,23,23	1.82	6 (30%)
3	GOL	H	501	-	5,5,5	0.52	0	5,5,5	0.60	0
2	PLP	E	500	-	16,16,16	2.94	5 (31%)	20,23,23	2.06	8 (40%)

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	PLP	F	500	-	-	1/8/8/8	0/1/1/1
3	GOL	B	504	-	-	2/4/4/4	-
3	GOL	F	501	-	-	2/4/4/4	-
3	GOL	H	504	-	-	2/4/4/4	-
3	GOL	E	504	-	-	2/4/4/4	-
2	PLP	A	500	-	-	2/8/8/8	0/1/1/1
3	GOL	G	504	-	-	1/4/4/4	-
3	GOL	A	504	-	-	4/4/4/4	-
2	PLP	G	500	-	-	2/8/8/8	0/1/1/1
3	GOL	C	501	-	-	2/4/4/4	-
2	PLP	D	500	-	-	5/8/8/8	0/1/1/1
3	GOL	A	501	-	-	0/4/4/4	-
2	PLP	C	500	-	-	5/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	H	500	-	-	4/8/8/8	0/1/1/1
3	GOL	C	504	-	-	0/4/4/4	-
2	PLP	B	500	-	-	3/8/8/8	0/1/1/1
3	GOL	H	501	-	-	0/4/4/4	-
2	PLP	E	500	-	-	3/8/8/8	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C3-C2	10.35	1.51	1.40
2	G	500	PLP	C3-C2	8.03	1.48	1.40
2	E	500	PLP	C3-C2	7.71	1.48	1.40
2	H	500	PLP	C3-C2	6.86	1.47	1.40
2	H	500	PLP	C4-C5	6.73	1.50	1.42
2	B	500	PLP	C3-C2	6.47	1.47	1.40
2	C	500	PLP	C4-C5	6.45	1.50	1.42
2	F	500	PLP	C3-C2	6.42	1.47	1.40
2	C	500	PLP	C3-C2	6.26	1.47	1.40
2	B	500	PLP	C4-C5	6.03	1.49	1.42
2	D	500	PLP	C3-C2	5.91	1.46	1.40
2	A	500	PLP	C4-C3	5.84	1.49	1.40
2	E	500	PLP	C4-C3	5.82	1.49	1.40
2	D	500	PLP	C4-C5	5.80	1.49	1.42
2	G	500	PLP	C4-C5	5.64	1.49	1.42
2	C	500	PLP	C4-C3	5.63	1.49	1.40
2	A	500	PLP	C4-C5	5.60	1.49	1.42
2	F	500	PLP	C4-C5	5.51	1.48	1.42
2	H	500	PLP	C4-C3	5.16	1.48	1.40
2	F	500	PLP	C4-C3	5.07	1.48	1.40
2	B	500	PLP	C4-C3	4.99	1.48	1.40
2	D	500	PLP	C4-C3	4.41	1.47	1.40
2	G	500	PLP	C4-C3	4.33	1.47	1.40
2	E	500	PLP	C4-C5	4.20	1.47	1.42
2	E	500	PLP	P-O2P	-3.43	1.41	1.54
2	C	500	PLP	P-O3P	-3.32	1.42	1.54
2	G	500	PLP	P-O3P	-2.91	1.43	1.54
2	D	500	PLP	P-O3P	-2.89	1.43	1.54
2	C	500	PLP	C6-N1	2.79	1.40	1.34
2	H	500	PLP	P-O3P	-2.77	1.44	1.54
2	B	500	PLP	P-O2P	-2.50	1.45	1.54
2	B	500	PLP	P-O4P	2.47	1.68	1.60
2	D	500	PLP	O3-C3	-2.47	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	PLP	P-O4P	2.47	1.68	1.60
2	D	500	PLP	C6-N1	2.36	1.39	1.34
2	F	500	PLP	P-O1P	-2.27	1.43	1.50
2	A	500	PLP	P-O3P	-2.26	1.46	1.54
2	G	500	PLP	P-O4P	2.20	1.67	1.60
2	E	500	PLP	O3-C3	-2.17	1.31	1.37
2	B	500	PLP	P-O1P	2.07	1.57	1.50
2	C	500	PLP	C2-N1	-2.04	1.30	1.33
2	B	500	PLP	O3-C3	-2.02	1.32	1.37

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	500	PLP	O4P-P-O1P	5.96	123.20	106.47
2	C	500	PLP	C6-N1-C2	5.06	128.53	119.17
2	C	500	PLP	O3P-P-O4P	4.98	119.98	106.73
2	D	500	PLP	O3P-P-O4P	4.86	119.66	106.73
2	E	500	PLP	O2P-P-O4P	4.52	118.76	106.73
2	G	500	PLP	O3P-P-O4P	4.47	118.62	106.73
2	G	500	PLP	C4-C3-C2	-4.34	117.50	120.19
2	A	500	PLP	O3P-P-O4P	4.32	118.23	106.73
2	A	500	PLP	C6-N1-C2	4.23	127.00	119.17
2	G	500	PLP	O4A-C4A-C4	-3.97	116.27	124.91
2	E	500	PLP	O4A-C4A-C4	-3.78	116.68	124.91
2	C	500	PLP	C4-C3-C2	-3.64	117.94	120.19
2	H	500	PLP	O3P-P-O4P	3.57	116.22	106.73
2	F	500	PLP	C6-N1-C2	3.56	125.76	119.17
2	F	500	PLP	C2A-C2-N1	3.54	124.59	117.67
2	B	500	PLP	O4A-C4A-C4	-3.39	117.53	124.91
2	E	500	PLP	C5A-C5-C6	3.29	124.79	119.37
2	B	500	PLP	O2P-P-O4P	3.26	115.40	106.73
2	F	500	PLP	O4A-C4A-C4	-3.23	117.88	124.91
2	A	500	PLP	C4-C3-C2	-3.22	118.20	120.19
2	G	500	PLP	C6-N1-C2	3.21	125.12	119.17
2	D	500	PLP	O4A-C4A-C4	-3.17	118.00	124.91
2	C	500	PLP	C3-C4-C5	2.98	120.54	118.26
2	F	500	PLP	C5A-C5-C6	2.87	124.09	119.37
2	G	500	PLP	O4P-P-O1P	-2.87	98.42	106.47
2	D	500	PLP	C6-N1-C2	2.86	124.47	119.17
2	A	500	PLP	C3-C2-N1	-2.85	117.09	120.77
2	D	500	PLP	C2A-C2-N1	2.85	123.23	117.67
2	C	500	PLP	O4A-C4A-C4	-2.84	118.72	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	PLP	C2A-C2-N1	2.83	123.20	117.67
2	F	500	PLP	O3P-P-O2P	2.80	118.33	107.64
2	C	500	PLP	C5A-C5-C6	2.72	123.85	119.37
2	B	500	PLP	C6-N1-C2	2.71	124.19	119.17
2	C	500	PLP	C3-C2-N1	-2.70	117.28	120.77
2	F	500	PLP	C3-C2-N1	-2.69	117.30	120.77
2	F	500	PLP	O2P-P-O1P	-2.67	100.22	110.68
2	E	500	PLP	C6-N1-C2	2.62	124.03	119.17
2	H	500	PLP	O4A-C4A-C4	-2.62	119.19	124.91
2	D	500	PLP	O3P-P-O2P	2.51	117.25	107.64
2	B	500	PLP	O4P-P-O1P	-2.51	99.42	106.47
2	F	500	PLP	O2P-P-O4P	-2.50	100.09	106.73
2	D	500	PLP	O4P-P-O1P	-2.49	99.48	106.47
2	A	500	PLP	O3P-P-O1P	2.46	120.31	110.68
2	D	500	PLP	O3P-P-O1P	-2.46	101.06	110.68
2	H	500	PLP	C6-N1-C2	2.45	123.71	119.17
2	B	500	PLP	C2A-C2-N1	2.42	122.40	117.67
2	D	500	PLP	C5A-C5-C6	2.40	123.32	119.37
2	A	500	PLP	O4A-C4A-C4	-2.36	119.78	124.91
2	H	500	PLP	C2A-C2-N1	2.31	122.19	117.67
2	F	500	PLP	C2A-C2-C3	-2.25	118.10	120.89
2	H	500	PLP	C3-C4-C5	-2.22	116.56	118.26
2	G	500	PLP	O3-C3-C2	2.18	122.23	117.49
2	E	500	PLP	O2P-P-O1P	2.17	119.18	110.68
2	E	500	PLP	O3P-P-O4P	-2.17	100.97	106.73
2	B	500	PLP	C5A-C5-C6	2.16	122.92	119.37
2	E	500	PLP	C2A-C2-N1	2.14	121.86	117.67
2	A	500	PLP	O4P-P-O1P	-2.10	100.57	106.47
2	H	500	PLP	O4P-P-O1P	-2.10	100.58	106.47
2	A	500	PLP	O3P-P-O2P	-2.09	99.64	107.64
3	C	501	GOL	O1-C1-C2	-2.08	100.24	110.20
2	D	500	PLP	C2A-C2-C3	-2.07	118.33	120.89
3	B	504	GOL	O3-C3-C2	-2.06	100.34	110.20
2	E	500	PLP	C3-C2-N1	-2.05	118.12	120.77
2	C	500	PLP	O4P-C5A-C5	2.04	113.23	109.35
2	G	500	PLP	C5-C6-N1	-2.02	120.45	123.82

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	PLP	C5A-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	C	500	PLP	C5A-O4P-P-O3P
2	D	500	PLP	C3-C4-C4A-O4A
2	D	500	PLP	C5A-O4P-P-O1P
2	D	500	PLP	C5A-O4P-P-O2P
2	D	500	PLP	C5A-O4P-P-O3P
3	A	504	GOL	O1-C1-C2-C3
3	C	501	GOL	C1-C2-C3-O3
3	E	504	GOL	C1-C2-C3-O3
3	F	501	GOL	O1-C1-C2-C3
3	H	504	GOL	O1-C1-C2-C3
2	C	500	PLP	C3-C4-C4A-O4A
2	H	500	PLP	C3-C4-C4A-O4A
2	E	500	PLP	C3-C4-C4A-O4A
2	F	500	PLP	C3-C4-C4A-O4A
3	A	504	GOL	C1-C2-C3-O3
3	B	504	GOL	C1-C2-C3-O3
2	A	500	PLP	C3-C4-C4A-O4A
2	B	500	PLP	C3-C4-C4A-O4A
2	G	500	PLP	C3-C4-C4A-O4A
3	C	501	GOL	O2-C2-C3-O3
3	F	501	GOL	O1-C1-C2-O2
3	H	504	GOL	O1-C1-C2-O2
2	A	500	PLP	C5-C4-C4A-O4A
3	B	504	GOL	O2-C2-C3-O3
2	C	500	PLP	C5A-O4P-P-O1P
3	G	504	GOL	C1-C2-C3-O3
3	A	504	GOL	O1-C1-C2-O2
3	E	504	GOL	O2-C2-C3-O3
2	B	500	PLP	C5A-O4P-P-O2P
2	E	500	PLP	C5A-O4P-P-O2P
2	D	500	PLP	C5-C4-C4A-O4A
2	G	500	PLP	C5-C4-C4A-O4A
2	H	500	PLP	C5A-O4P-P-O1P
2	B	500	PLP	C5-C4-C4A-O4A
2	C	500	PLP	C5-C4-C4A-O4A
3	A	504	GOL	O2-C2-C3-O3
2	H	500	PLP	C5A-O4P-P-O3P
2	E	500	PLP	C5-C4-C4A-O4A
2	H	500	PLP	C5-C4-C4A-O4A

There are no ring outliers.

14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	PLP	1	0
3	B	504	GOL	3	0
3	H	504	GOL	1	0
3	E	504	GOL	2	0
2	A	500	PLP	6	0
3	G	504	GOL	1	0
3	A	504	GOL	1	0
2	G	500	PLP	4	0
2	D	500	PLP	3	0
2	C	500	PLP	1	0
2	H	500	PLP	1	0
3	C	504	GOL	7	0
2	B	500	PLP	1	0
2	E	500	PLP	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	436/448 (97%)	-0.23	0 100 100	7, 13, 24, 64	0
1	B	435/448 (97%)	-0.37	1 (0%) 95 94	7, 14, 22, 64	0
1	C	436/448 (97%)	-0.43	0 100 100	6, 11, 21, 63	0
1	D	436/448 (97%)	-0.37	1 (0%) 95 94	6, 12, 21, 76	0
1	E	435/448 (97%)	-0.46	1 (0%) 95 94	7, 11, 20, 75	0
1	F	436/448 (97%)	-0.24	2 (0%) 91 91	6, 12, 22, 76	0
1	G	436/448 (97%)	-0.26	1 (0%) 95 94	8, 15, 26, 83	0
1	H	436/448 (97%)	-0.10	4 (0%) 84 85	7, 16, 32, 91	0
All	All	3486/3584 (97%)	-0.31	10 (0%) 94 94	6, 13, 25, 91	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	13	SER	4.2
1	H	13	SER	4.0
1	D	13	SER	4.0
1	H	367	GLY	3.0
1	E	14	GLU	2.9
1	H	448	ALA	2.7
1	B	14	GLU	2.4
1	F	13	SER	2.3
1	F	370[A]	GLY	2.1
1	H	388[A]	ILE	2.1

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	PLP	A	500	16/16	0.91	0.18	9,16,23,28	16
2	PLP	B	500	16/16	0.91	0.16	8,17,21,37	16
3	GOL	G	504	6/6	0.91	0.15	18,27,38,46	0
3	GOL	C	504	6/6	0.92	0.15	13,19,31,32	0
2	PLP	D	500	16/16	0.92	0.17	6,15,20,30	16
3	GOL	H	501	6/6	0.92	0.12	18,20,25,29	0
2	PLP	C	500	16/16	0.93	0.16	5,13,18,28	16
3	GOL	F	501	6/6	0.93	0.15	15,22,30,34	0
2	PLP	F	500	16/16	0.93	0.15	7,14,18,23	16
2	PLP	G	500	16/16	0.93	0.17	9,17,24,46	16
3	GOL	H	504	6/6	0.93	0.17	14,21,29,30	0
3	GOL	C	501	6/6	0.94	0.15	17,25,32,52	0
2	PLP	E	500	16/16	0.94	0.18	6,14,18,29	16
2	PLP	H	500	16/16	0.94	0.15	11,19,25,33	16
3	GOL	A	504	6/6	0.95	0.16	14,27,38,43	0
3	GOL	E	504	6/6	0.95	0.12	12,18,28,35	0
3	GOL	A	501	6/6	0.95	0.11	13,14,20,25	0
3	GOL	B	504	6/6	0.96	0.15	15,32,38,39	0
4	CL	G	502	1/1	0.96	0.05	22,22,22,22	0
4	CL	C	502	1/1	0.98	0.06	13,13,13,13	0
4	CL	A	502	1/1	0.99	0.05	14,14,14,14	0
4	CL	D	502	1/1	0.99	0.05	18,18,18,18	0
4	CL	E	502	1/1	0.99	0.04	18,18,18,18	0
4	CL	F	502	1/1	0.99	0.04	14,14,14,14	0
4	CL	B	502	1/1	0.99	0.04	18,18,18,18	0
4	CL	H	502	1/1	0.99	0.05	16,16,16,16	0
5	CA	E	503	1/1	0.99	0.04	17,17,17,17	0
5	CA	H	503	1/1	0.99	0.05	19,19,19,19	0
5	CA	G	503	1/1	1.00	0.06	20,20,20,20	0
5	CA	F	503	1/1	1.00	0.09	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.