Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 04:09 pm GMT

PDB ID	:	4BPT
Title	:	Structural and thermodynamic insight into phenylalanine hydroxylase from the human pathogen Legionella pneumophila
Authors	:	Leiros, H.-K.S.; Flydal, M.I.; Martinez, A.
Deposited on	:	2013-05-28
Resolution	:	2.50 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:

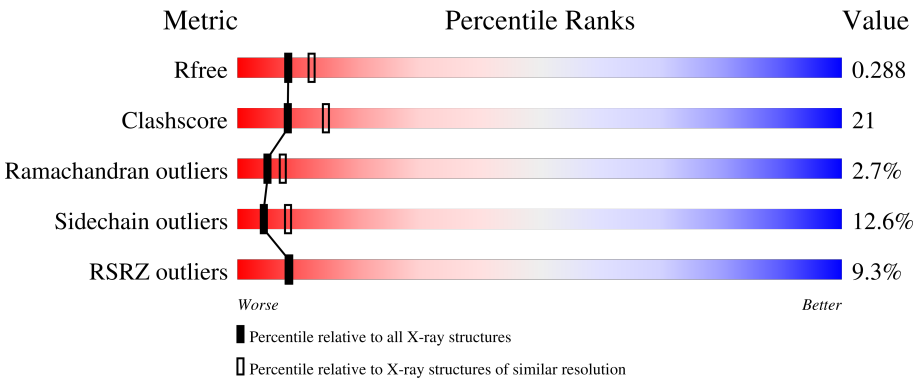
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	272	57% 26% 8% • 7%
1	B	272	56% 26% 8% • 7%
1	C	272	17% 45% 29% 8% • 15%
1	D	272	15% 50% 26% 8% • 13%

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	PEG	A	1260	-	-	X	-
2	PEG	A	1261	-	-	X	-
2	PEG	A	1262	-	-	X	-
2	PEG	B	1260	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8155 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.

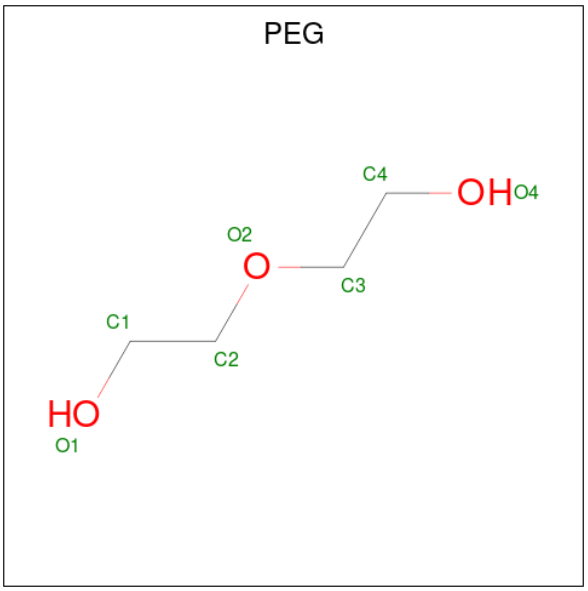
- Molecule 1 is a protein called PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	2062	1345	331	377	9	5	1	0
1	B	252	2053	1340	330	374	9	10	0	0
1	C	232	1900	1246	302	343	9	193	0	0
1	D	237	1943	1272	311	351	9	135	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	THR	ILE	conflict	UNP I7HM43
B	60	THR	ILE	conflict	UNP I7HM43
C	60	THR	ILE	conflict	UNP I7HM43
D	60	THR	ILE	conflict	UNP I7HM43

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 3 is water.

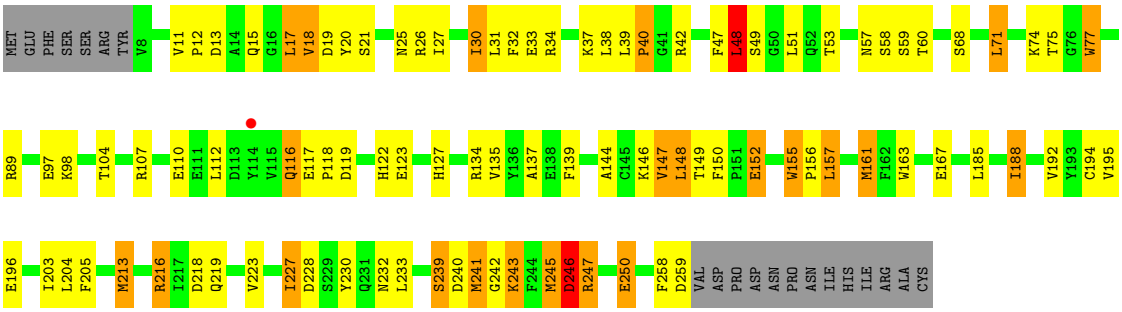
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	56	56	56	0	0
			Total	O		
3	B	51	51	51	0	0
			Total	O		
3	C	27	27	27	0	0
			Total	O		
3	D	21	21	21	0	0

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.

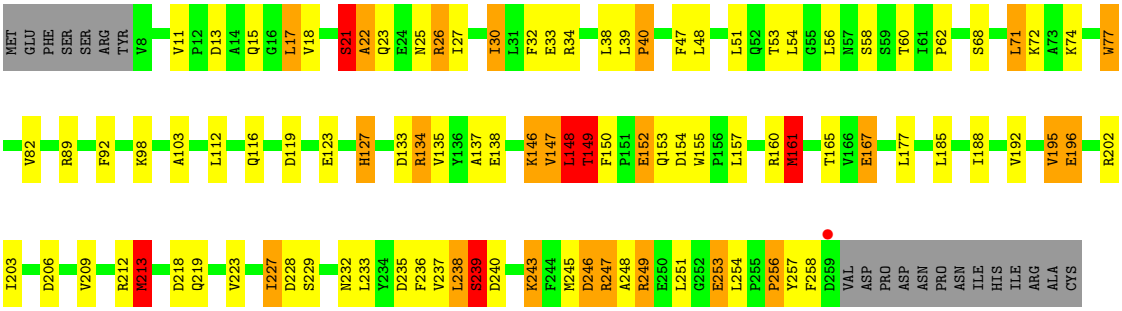
• Molecule 1: PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)

Chain A:



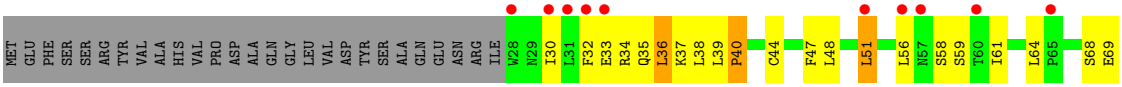
• Molecule 1: PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)

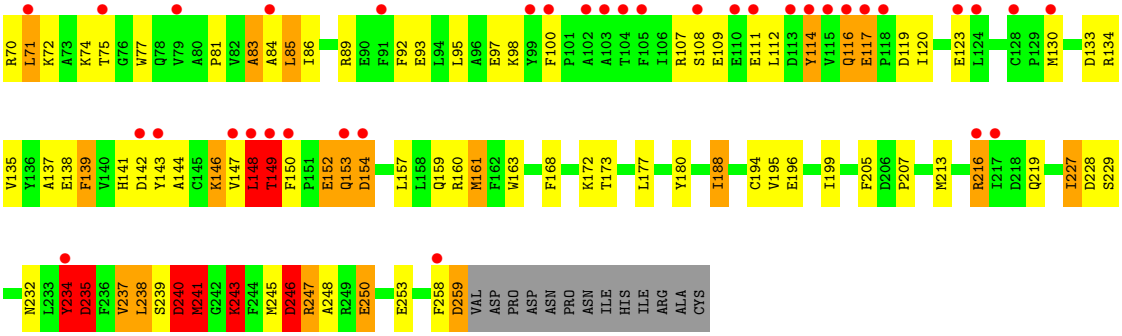
Chain B:



• Molecule 1: PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)

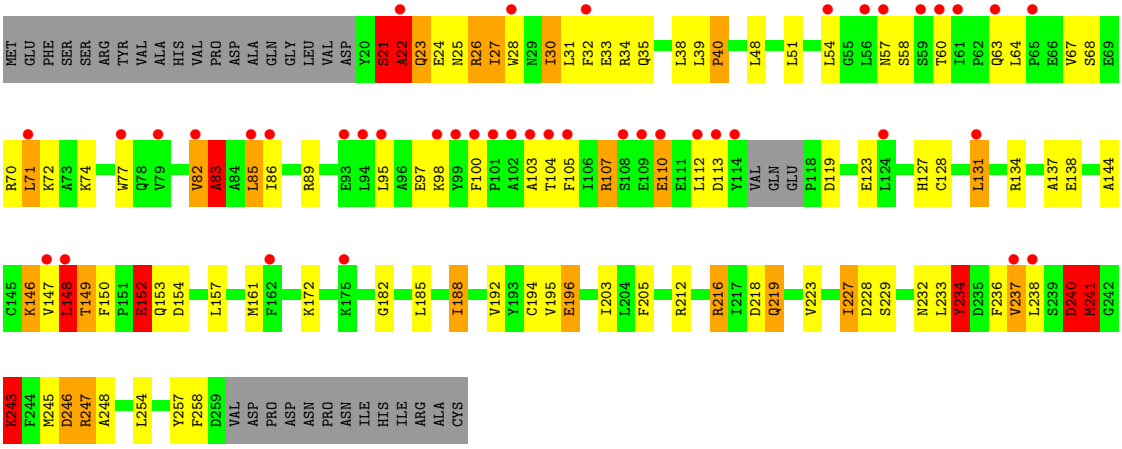
Chain C:





• Molecule 1: PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.32Å 60.12Å 124.04Å 90.00° 94.07° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 24.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.4 (10.00-2.50) 90.3 (24.32-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.264 , 0.302 0.252 , 0.288	Depositor DCC
R_{free} test set	1291 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8155	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.43% 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: PEG

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	1.44	6/2121 (0.3%)	1.14	11/2885 (0.4%)
1	B	1.70	9/2112 (0.4%)	1.24	16/2873 (0.6%)
1	C	2.82	48/1956 (2.5%)	2.67	78/2659 (2.9%)
1	D	2.11	32/1999 (1.6%)	1.99	44/2714 (1.6%)
All	All	2.07	95/8188 (1.2%)	1.84	149/11131 (1.3%)

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	B	1	4
1	C	1	6
1	D	0	6
All	All	2	17

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	GLU	CG-CD	-48.09	0.79	1.51
1	B	239	SER	CB-OG	-45.23	0.83	1.42
1	A	110	GLU	CB-CG	37.99	2.24	1.52
1	D	63	GLN	CG-CD	37.46	2.37	1.51
1	C	146	LYS	CE-NZ	33.07	2.31	1.49
1	C	92	PHE	CB-CG	-32.89	0.95	1.51
1	C	149	THR	CB-CG2	30.81	2.54	1.52
1	C	246	ASP	CB-CG	29.20	2.13	1.51
1	C	109	GLU	C-N	-28.81	0.67	1.34
1	B	21	SER	CA-CB	-28.59	1.10	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	GLU	CB-CG	28.33	2.06	1.52
1	D	85	LEU	CB-CG	28.14	2.34	1.52
1	C	234	TYR	CE2-CZ	-26.33	1.04	1.38
1	C	81	PRO	C-N	-25.85	0.74	1.34
1	C	111	GLU	CB-CG	24.25	1.98	1.52
1	C	112	LEU	CB-CG	-23.18	0.85	1.52
1	C	148	LEU	CB-CG	-22.09	0.88	1.52
1	D	27	ILE	CA-CB	22.09	2.05	1.54
1	B	253	GLU	CD-OE1	-20.95	1.02	1.25
1	D	21	SER	CA-CB	-20.89	1.21	1.52
1	D	57	ASN	CA-CB	19.98	2.05	1.53
1	C	69	GLU	CA-CB	19.88	1.97	1.53
1	C	234	TYR	CZ-OH	18.95	1.70	1.37
1	D	110	GLU	CB-CG	18.85	1.88	1.52
1	D	234	TYR	CD1-CE1	18.75	1.67	1.39
1	C	139	PHE	CD1-CE1	-17.84	1.03	1.39
1	C	108	SER	C-N	17.83	1.75	1.34
1	A	239	SER	CB-OG	-17.66	1.19	1.42
1	D	107	ARG	CD-NE	-17.36	1.17	1.46
1	D	138	GLU	CG-CD	17.00	1.77	1.51
1	C	72	LYS	CB-CG	16.82	1.98	1.52
1	D	104	THR	CA-CB	16.42	1.96	1.53
1	D	234	TYR	CE2-CZ	15.96	1.59	1.38
1	D	74	LYS	CA-CB	-15.86	1.19	1.53
1	C	139	PHE	CG-CD2	-14.81	1.16	1.38
1	D	105	PHE	CB-CG	-14.46	1.26	1.51
1	D	82	VAL	C-N	14.07	1.66	1.34
1	C	234	TYR	CB-CG	-13.87	1.30	1.51
1	C	134	ARG	CA-CB	13.25	1.83	1.53
1	D	26	ARG	CA-CB	12.63	1.81	1.53
1	C	89	ARG	CB-CG	-12.00	1.20	1.52
1	C	74	LYS	CA-CB	-11.67	1.28	1.53
1	D	218	ASP	CG-OD1	11.53	1.51	1.25
1	C	259	ASP	CA-CB	-11.24	1.29	1.53
1	C	85	LEU	CB-CG	11.12	1.84	1.52
1	C	234	TYR	CG-CD2	-11.09	1.24	1.39
1	C	61	ILE	CB-CG2	-10.99	1.18	1.52
1	C	149	THR	CB-OG1	-10.97	1.21	1.43
1	C	153	GLN	CG-CD	-10.51	1.26	1.51
1	D	64	LEU	CA-CB	10.11	1.77	1.53
1	C	83	ALA	C-N	9.89	1.56	1.34
1	D	134	ARG	CG-CD	9.63	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	239	SER	CB-OG	9.12	1.54	1.42
1	C	37	LYS	CB-CG	-8.99	1.28	1.52
1	C	116	GLN	CG-CD	-8.84	1.30	1.51
1	C	36	LEU	CA-CB	-8.72	1.33	1.53
1	C	146	LYS	CG-CD	-8.68	1.23	1.52
1	C	250	GLU	CB-CG	-8.56	1.35	1.52
1	C	86	ILE	CA-CB	8.46	1.74	1.54
1	D	67	VAL	CB-CG2	-8.15	1.35	1.52
1	D	153	GLN	CG-CD	7.96	1.69	1.51
1	D	146	LYS	CB-CG	-7.93	1.31	1.52
1	C	64	LEU	CA-CB	-7.89	1.35	1.53
1	C	97	GLU	CB-CG	-7.66	1.37	1.52
1	D	218	ASP	CG-OD2	-7.50	1.08	1.25
1	B	77	TRP	CD2-CE2	7.21	1.50	1.41
1	D	83	ALA	C-N	-7.11	1.17	1.34
1	B	149	THR	CB-OG1	6.88	1.57	1.43
1	C	59	SER	CA-CB	6.87	1.63	1.52
1	D	95	LEU	CB-CG	6.87	1.72	1.52
1	D	152	GLU	CD-OE2	-6.86	1.18	1.25
1	D	54	LEU	CB-CG	-6.80	1.32	1.52
1	C	141	HIS	CA-CB	6.75	1.68	1.53
1	D	70	ARG	CB-CG	-6.62	1.34	1.52
1	B	167	GLU	CD-OE2	-6.61	1.18	1.25
1	C	100	PHE	CA-CB	-6.51	1.39	1.53
1	A	77	TRP	CD2-CE2	6.50	1.49	1.41
1	A	49	SER	CB-OG	-6.23	1.34	1.42
1	C	93	GLU	CB-CG	-6.11	1.40	1.52
1	C	240	ASP	CG-OD2	6.09	1.39	1.25
1	C	56	LEU	CB-CG	6.05	1.70	1.52
1	C	120	ILE	CB-CG2	-6.00	1.34	1.52
1	C	97	GLU	CG-CD	5.85	1.60	1.51
1	A	167	GLU	CD-OE2	-5.72	1.19	1.25
1	C	107	ARG	CB-CG	-5.67	1.37	1.52
1	B	155	TRP	CD2-CE2	5.65	1.48	1.41
1	D	243	LYS	CA-CB	5.64	1.66	1.53
1	C	253	GLU	CB-CG	5.58	1.62	1.52
1	D	196	GLU	CG-CD	5.49	1.60	1.51
1	B	22	ALA	N-CA	5.40	1.57	1.46
1	C	51	LEU	CG-CD2	-5.39	1.31	1.51
1	D	241	MET	SD-CE	-5.38	1.47	1.77
1	D	28	TRP	CD2-CE2	5.13	1.47	1.41
1	A	155	TRP	CD2-CE2	5.04	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	HIS	CG-CD2	5.01	1.44	1.35

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	83	ALA	O-C-N	-38.34	61.35	122.70
1	C	234	TYR	CB-CG-CD2	34.79	141.88	121.00
1	C	117	GLU	CG-CD-OE1	-31.88	54.55	118.30
1	D	234	TYR	CG-CD1-CE1	-29.91	97.37	121.30
1	D	107	ARG	CD-NE-CZ	-29.57	82.20	123.60
1	D	22	ALA	O-C-N	-28.21	77.56	122.70
1	C	148	LEU	CA-CB-CG	27.43	178.40	115.30
1	D	234	TYR	CE1-CZ-CE2	-27.24	76.22	119.80
1	C	112	LEU	CB-CG-CD2	-26.55	65.86	111.00
1	C	148	LEU	CB-CG-CD2	24.66	152.92	111.00
1	D	218	ASP	CB-CG-OD2	23.69	139.62	118.30
1	C	83	ALA	CA-C-N	23.47	168.83	117.20
1	C	112	LEU	CB-CG-CD1	23.14	150.34	111.00
1	C	146	LYS	CD-CE-NZ	-23.01	58.77	111.70
1	C	97	GLU	CA-CB-CG	22.86	163.70	113.40
1	D	107	ARG	CG-CD-NE	-21.64	66.34	111.80
1	C	117	GLU	CG-CD-OE2	20.95	160.20	118.30
1	C	109	GLU	O-C-N	20.36	155.27	122.70
1	C	149	THR	CA-CB-CG2	-20.11	84.25	112.40
1	C	92	PHE	CB-CG-CD2	-18.30	107.99	120.80
1	D	218	ASP	CB-CG-OD1	-17.91	102.18	118.30
1	C	139	PHE	CG-CD1-CE1	17.59	140.15	120.80
1	C	149	THR	OG1-CB-CG2	-17.43	69.91	110.00
1	B	21	SER	N-CA-CB	17.39	136.59	110.50
1	C	81	PRO	O-C-N	-16.14	96.88	122.70
1	C	153	GLN	CG-CD-OE1	15.95	153.50	121.60
1	C	109	GLU	CA-C-N	-15.90	82.23	117.20
1	C	234	TYR	CG-CD2-CE2	15.77	133.91	121.30
1	C	92	PHE	CB-CG-CD1	15.61	131.73	120.80
1	C	61	ILE	CG1-CB-CG2	15.42	145.32	111.40
1	C	75	THR	CA-CB-CG2	-14.76	91.74	112.40
1	D	234	TYR	CD1-CE1-CZ	14.71	133.03	119.80
1	C	85	LEU	CB-CG-CD2	-14.61	86.16	111.00
1	C	234	TYR	CB-CG-CD1	-14.45	112.33	121.00
1	C	117	GLU	CB-CG-CD	-14.11	76.12	114.20
1	D	54	LEU	CB-CG-CD1	-14.09	87.04	111.00
1	D	26	ARG	N-CA-CB	-14.05	85.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	153	GLN	CG-CD-NE2	-13.97	83.18	116.70
1	D	98	LYS	CA-CB-CG	-13.60	83.48	113.40
1	C	241	MET	CG-SD-CE	13.05	121.09	100.20
1	C	139	PHE	CD1-CE1-CZ	-13.04	104.45	120.10
1	D	105	PHE	CB-CG-CD2	-12.94	111.74	120.80
1	D	153	GLN	CG-CD-OE1	12.86	147.32	121.60
1	A	110	GLU	CA-CB-CG	-12.81	85.21	113.40
1	C	154	ASP	CB-CG-OD2	12.78	129.81	118.30
1	D	105	PHE	CB-CG-CD1	12.72	129.70	120.80
1	C	259	ASP	N-CA-CB	12.64	133.36	110.60
1	C	97	GLU	CB-CG-CD	12.47	147.86	114.20
1	D	153	GLN	CG-CD-NE2	-12.42	86.88	116.70
1	C	81	PRO	CA-C-N	12.21	144.05	117.20
1	C	240	ASP	CB-CG-OD2	-12.15	107.37	118.30
1	C	154	ASP	CB-CG-OD1	-12.11	107.40	118.30
1	C	59	SER	N-CA-CB	12.08	128.62	110.50
1	D	21	SER	CA-CB-OG	-11.97	78.89	111.20
1	C	234	TYR	CD1-CG-CD2	-11.75	104.98	117.90
1	D	234	TYR	CZ-CE2-CD2	-11.58	109.38	119.80
1	D	54	LEU	CA-CB-CG	-11.52	88.79	115.30
1	C	108	SER	CA-C-N	-11.46	91.99	117.20
1	D	85	LEU	CB-CG-CD2	-11.05	92.22	111.00
1	C	116	GLN	CB-CG-CD	-10.87	83.33	111.60
1	C	148	LEU	CB-CG-CD1	-10.86	92.53	111.00
1	D	86	ILE	CA-CB-CG1	-10.72	90.63	111.00
1	B	161	MET	CG-SD-CE	-10.61	83.23	100.20
1	C	246	ASP	CB-CG-OD2	-10.56	108.79	118.30
1	D	21	SER	CB-CA-C	-10.36	90.41	110.10
1	D	67	VAL	CG1-CB-CG2	10.35	127.47	110.90
1	D	86	ILE	CA-CB-CG2	-10.16	90.57	110.90
1	C	74	LYS	N-CA-CB	-10.03	92.54	110.60
1	B	26	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	C	134	ARG	N-CA-CB	-9.83	92.90	110.60
1	B	26	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	C	56	LEU	CB-CG-CD2	9.60	127.32	111.00
1	C	239	SER	CA-CB-OG	-9.55	85.41	111.20
1	C	70	ARG	CB-CG-CD	9.15	135.39	111.60
1	D	97	GLU	CA-CB-CG	9.12	133.47	113.40
1	C	81	PRO	C-N-CA	9.09	144.43	121.70
1	A	26	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	A	26	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	C	95	LEU	CB-CG-CD1	-8.79	96.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	86	ILE	CB-CG1-CD1	-8.41	90.35	113.90
1	C	234	TYR	CA-CB-CG	8.41	129.37	113.40
1	B	253	GLU	CG-CD-OE1	-8.10	102.11	118.30
1	D	83	ALA	C-N-CA	-8.10	101.46	121.70
1	C	93	GLU	CA-CB-CG	8.04	131.10	113.40
1	D	26	ARG	CB-CA-C	7.93	126.27	110.40
1	A	110	GLU	CB-CG-CD	7.83	135.35	114.20
1	D	57	ASN	CB-CA-C	-7.79	94.82	110.40
1	C	70	ARG	CG-CD-NE	7.73	128.03	111.80
1	C	83	ALA	C-N-CA	7.66	140.84	121.70
1	C	154	ASP	CA-CB-CG	7.53	129.97	113.40
1	C	240	ASP	OD1-CG-OD2	-7.51	109.03	123.30
1	D	27	ILE	CA-CB-CG2	-7.46	95.98	110.90
1	C	85	LEU	CB-CG-CD1	7.40	123.58	111.00
1	D	67	VAL	CA-CB-CG2	7.36	121.94	110.90
1	D	74	LYS	CA-CB-CG	-7.35	97.24	113.40
1	C	243	LYS	CG-CD-CE	-7.24	90.18	111.90
1	C	120	ILE	CG1-CB-CG2	-7.24	95.48	111.40
1	C	72	LYS	CA-CB-CG	7.22	129.27	113.40
1	B	256	PRO	N-CA-C	7.11	130.58	112.10
1	C	108	SER	C-N-CA	-7.11	103.93	121.70
1	D	23	GLN	O-C-N	-7.05	111.42	122.70
1	D	110	GLU	CB-CG-CD	6.98	133.03	114.20
1	D	54	LEU	CB-CG-CD2	-6.93	99.22	111.00
1	D	63	GLN	CB-CG-CD	-6.92	93.61	111.60
1	C	51	LEU	CB-CG-CD2	6.90	122.73	111.00
1	D	74	LYS	CB-CA-C	-6.89	96.62	110.40
1	D	152	GLU	CG-CD-OE1	-6.82	104.67	118.30
1	C	74	LYS	CB-CA-C	6.74	123.88	110.40
1	C	72	LYS	CB-CG-CD	6.71	129.06	111.60
1	A	233	LEU	CB-CG-CD2	-6.68	99.65	111.00
1	C	246	ASP	CA-CB-CG	-6.50	99.11	113.40
1	B	238	LEU	N-CA-C	-6.41	93.69	111.00
1	B	21	SER	CA-CB-OG	6.40	128.48	111.20
1	C	139	PHE	CG-CD2-CE2	-6.40	113.76	120.80
1	C	238	LEU	N-CA-C	-6.40	93.73	111.00
1	C	109	GLU	C-N-CA	-6.30	105.96	121.70
1	C	120	ILE	CA-CB-CG2	6.28	123.47	110.90
1	C	95	LEU	CA-CB-CG	-6.25	100.93	115.30
1	B	249	ARG	CB-CA-C	6.19	122.79	110.40
1	C	235	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	93	GLU	CB-CG-CD	6.17	130.87	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	SER	CA-CB-OG	6.16	127.84	111.20
1	C	61	ILE	CA-CB-CG1	-6.14	99.34	111.00
1	B	213	MET	CG-SD-CE	-6.12	90.42	100.20
1	D	97	GLU	CB-CG-CD	6.09	130.64	114.20
1	C	51	LEU	CD1-CG-CD2	5.88	128.15	110.50
1	D	95	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	C	259	ASP	CA-CB-CG	5.78	126.12	113.40
1	A	148	LEU	N-CA-CB	5.77	121.93	110.40
1	A	104	THR	CA-CB-CG2	-5.73	104.38	112.40
1	B	196	GLU	CB-CA-C	-5.65	99.09	110.40
1	A	48	LEU	CB-CG-CD2	5.62	120.55	111.00
1	D	22	ALA	CA-C-N	5.59	129.50	117.20
1	D	85	LEU	CB-CG-CD1	5.57	120.47	111.00
1	C	112	LEU	CA-CB-CG	-5.56	102.50	115.30
1	A	97	GLU	CA-CB-CG	5.45	125.40	113.40
1	D	71	LEU	CA-CB-CG	-5.39	102.89	115.30
1	C	36	LEU	CB-CA-C	5.33	120.32	110.20
1	B	235	ASP	CB-CG-OD1	5.28	123.06	118.30
1	A	246	ASP	N-CA-C	-5.25	96.83	111.00
1	B	165	THR	CA-CB-CG2	-5.25	105.06	112.40
1	B	249	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	75	THR	OG1-CB-CG2	5.14	121.83	110.00
1	C	74	LYS	CA-CB-CG	5.14	124.71	113.40
1	C	235	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	D	21	SER	N-CA-CB	5.08	118.12	110.50
1	D	134	ARG	CB-CG-CD	-5.08	98.38	111.60
1	B	146	LYS	CD-CE-NZ	-5.01	100.18	111.70
1	B	134	ARG	NE-CZ-NH1	-5.00	117.80	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	21	SER	CA
1	C	259	ASP	CA

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	VAL	Peptide
1	B	147	VAL	Peptide
1	B	148	LEU	Peptide
1	B	21	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	253	GLU	Sidechain
1	C	148	LEU	Peptide
1	C	240	ASP	Sidechain
1	C	241	MET	Peptide
1	C	246	ASP	Sidechain
1	C	83	ALA	Peptide,Mainchain
1	D	148	LEU	Peptide
1	D	22	ALA	Mainchain
1	D	23	GLN	Peptide
1	D	234	TYR	Sidechain
1	D	240	ASP	Peptide
1	D	83	ALA	Mainchain

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	2062	0	2010	87	0
1	B	2053	0	2005	89	0
1	C	1900	0	1857	67	0
1	D	1943	0	1900	59	0
2	A	21	0	30	14	0
2	B	21	0	30	8	0
3	A	56	0	0	5	0
3	B	51	0	0	13	0
3	C	27	0	0	3	0
3	D	21	0	0	0	0
All	All	8155	0	7832	316	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 (316) 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:44:CYS:SG	1:C:130:MET:HE1	1.57	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:CYS:SG	1:C:130:MET:CE	2.13	1.34
1:B:26:ARG:N	3:B:2006:HOH:O	1.71	1.21
1:B:27:ILE:N	3:B:2006:HOH:O	1.73	1.19
1:C:240:ASP:HA	1:C:241:MET:HB2	1.24	1.19
1:A:127:HIS:NE2	3:A:2032:HOH:O	1.76	1.12
1:B:177:LEU:HD23	1:B:195:VAL:HG12	1.32	1.11
1:A:30:ILE:HD11	1:A:112:LEU:HD21	1.25	1.07
1:B:30:ILE:HD11	1:B:112:LEU:HD21	1.08	1.06
1:D:194:CYS:SG	1:D:195:VAL:HG13	1.96	1.04
1:A:148:LEU:O	1:A:149:THR:HB	1.49	1.04
1:C:240:ASP:HB2	1:C:241:MET:HB3	1.42	1.00
1:C:44:CYS:SG	1:C:130:MET:HE3	1.96	0.99
1:C:142:ASP:OD2	1:C:237:VAL:HG11	1.62	0.99
1:D:236:PHE:O	1:D:237:VAL:HG22	1.60	0.99
2:A:1262:PEG:H11	2:A:1262:PEG:H42	1.42	0.98
1:A:25:ASN:ND2	1:A:60:THR:HG22	1.79	0.97
1:C:142:ASP:CG	1:C:237:VAL:HG11	1.84	0.97
1:D:212:ARG:HB3	1:D:254:LEU:HD13	1.46	0.96
1:C:240:ASP:HA	1:C:241:MET:CB	1.96	0.96
2:A:1262:PEG:H42	2:A:1262:PEG:C1	1.93	0.96
1:B:30:ILE:CD1	1:B:112:LEU:HD21	1.96	0.93
1:B:25:ASN:HD22	1:B:60:THR:HA	1.37	0.90
1:A:149:THR:HG21	3:A:2036:HOH:O	1.73	0.89
1:B:212:ARG:HB3	1:B:254:LEU:HD13	1.55	0.88
1:A:163:TRP:HZ3	2:A:1261:PEG:H22	1.41	0.86
1:A:148:LEU:O	1:A:149:THR:CB	2.19	0.85
1:B:202:ARG:HD2	3:B:2040:HOH:O	1.75	0.85
2:B:1260:PEG:H42	2:B:1260:PEG:O1	1.76	0.85
1:B:148:LEU:O	1:B:149:THR:HG22	1.77	0.84
1:C:142:ASP:OD2	1:C:237:VAL:CG1	2.25	0.84
1:C:240:ASP:CA	1:C:241:MET:CB	2.56	0.83
1:B:153:GLN:HG3	3:B:2033:HOH:O	1.77	0.82
1:B:25:ASN:ND2	1:B:60:THR:HA	1.93	0.82
1:C:240:ASP:CA	1:C:241:MET:HB2	2.09	0.81
1:A:30:ILE:CD1	1:A:112:LEU:HD21	2.10	0.81
1:B:240:ASP:OD2	1:B:243:LYS:HB2	1.80	0.80
1:D:25:ASN:ND2	1:D:60:THR:HG22	1.97	0.79
1:A:25:ASN:HD22	1:A:60:THR:HG22	1.46	0.79
1:D:128:CYS:HA	1:D:131:LEU:HD22	1.62	0.79
1:D:25:ASN:HD22	1:D:60:THR:HG22	1.49	0.78
1:C:240:ASP:CB	1:C:241:MET:HB3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:HD13	1:B:77:TRP:HB3	1.65	0.77
1:A:127:HIS:CE1	3:A:2032:HOH:O	2.28	0.77
1:D:31:LEU:HD11	1:D:107:ARG:HD2	1.65	0.77
1:D:234:TYR:O	1:D:238:LEU:HD13	1.85	0.76
1:C:243:LYS:O	1:C:246:ASP:O	2.04	0.76
1:A:247:ARG:HA	1:A:250[B]:GLU:HG2	1.67	0.76
1:B:161:MET:HE3	1:B:161:MET:O	1.85	0.75
1:B:161:MET:HE3	1:B:161:MET:C	2.06	0.75
1:B:148:LEU:C	1:B:149:THR:HG22	2.07	0.74
1:A:161:MET:C	1:A:161:MET:HE3	2.06	0.74
1:D:243:LYS:O	1:D:246:ASP:O	2.05	0.74
1:B:25:ASN:ND2	1:B:60:THR:HG22	2.03	0.73
1:A:146:LYS:O	1:A:148:LEU:O	2.08	0.72
1:B:243:LYS:O	1:B:246:ASP:O	2.07	0.72
2:A:1261:PEG:H11	2:A:1262:PEG:H12	1.72	0.71
2:A:1260:PEG:H22	2:A:1262:PEG:O4	1.90	0.71
1:A:194:CYS:SG	1:A:195:VAL:HG13	2.31	0.70
1:A:243:LYS:O	1:A:246:ASP:O	2.08	0.70
1:A:57:ASN:ND2	1:A:59:SER:HB3	2.07	0.69
1:A:163:TRP:CZ3	2:A:1261:PEG:H22	2.26	0.69
1:B:153:GLN:CB	3:B:2033:HOH:O	2.41	0.69
1:C:228:ASP:H	1:C:232:ASN:ND2	1.91	0.69
1:A:148:LEU:C	1:A:150:PHE:H	1.95	0.69
1:C:228:ASP:H	1:C:232:ASN:HD21	1.41	0.69
1:C:138:GLU:OE1	3:C:2014:HOH:O	2.11	0.68
1:D:212:ARG:HB3	1:D:254:LEU:CD1	2.23	0.68
1:C:148:LEU:O	1:C:149:THR:HB	1.92	0.68
1:A:150:PHE:CE1	1:A:245:MET:HE1	2.30	0.67
1:D:212:ARG:CZ	1:D:254:LEU:HD11	2.24	0.67
1:A:161:MET:HE3	1:A:161:MET:O	1.94	0.67
1:B:177:LEU:HD23	1:B:195:VAL:CG1	2.20	0.66
2:A:1261:PEG:H11	2:A:1262:PEG:C1	2.25	0.66
1:B:177:LEU:CD2	1:B:195:VAL:HG12	2.20	0.66
1:C:142:ASP:OD1	1:C:237:VAL:HG11	1.95	0.65
2:B:1260:PEG:O4	2:B:1262:PEG:H22	1.96	0.65
1:D:203:ILE:HD12	1:D:223:VAL:HG13	1.76	0.65
1:B:25:ASN:ND2	1:B:60:THR:CA	2.59	0.65
1:D:236:PHE:O	1:D:237:VAL:CG2	2.42	0.65
1:C:234:TYR:OH	1:C:234:TYR:CE2	2.49	0.64
1:B:25:ASN:HD22	1:B:60:THR:HG22	1.62	0.64
2:B:1260:PEG:C1	2:B:1260:PEG:C4	2.73	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASP:O	1:A:247:ARG:CB	2.46	0.64
2:B:1260:PEG:H42	2:B:1260:PEG:C1	2.28	0.63
1:D:227:ILE:HG23	1:D:229:SER:H	1.63	0.63
1:A:228:ASP:H	1:A:232:ASN:HD21	1.47	0.62
1:B:238:LEU:O	1:B:239:SER:CB	2.44	0.62
1:B:212:ARG:CB	1:B:254:LEU:HD13	2.28	0.62
1:A:242:GLY:H	1:A:245:MET:HE2	1.65	0.62
1:B:228:ASP:H	1:B:232:ASN:ND2	1.98	0.62
1:B:246:ASP:O	1:B:247:ARG:CB	2.48	0.62
1:A:228:ASP:H	1:A:232:ASN:ND2	1.98	0.61
1:B:18:VAL:HG23	3:B:2003:HOH:O	1.99	0.61
1:B:25:ASN:HD22	1:B:60:THR:CA	2.12	0.61
1:B:148:LEU:O	1:B:149:THR:CG2	2.48	0.61
1:B:212:ARG:HB3	1:B:254:LEU:CD1	2.28	0.61
2:B:1260:PEG:O1	2:B:1260:PEG:C4	2.49	0.61
1:B:246:ASP:O	1:B:247:ARG:HB3	2.02	0.60
1:A:246:ASP:O	1:A:247:ARG:HB3	2.01	0.60
1:D:246:ASP:O	1:D:247:ARG:CB	2.48	0.60
1:C:227:ILE:HG23	1:C:229:SER:H	1.67	0.60
1:C:235:ASP:CG	3:C:2021:HOH:O	2.39	0.60
1:B:206:ASP:OD2	1:B:209:VAL:HG23	2.02	0.59
1:D:246:ASP:O	1:D:247:ARG:HB3	2.02	0.59
1:A:18:VAL:HG21	1:A:20:TYR:CZ	2.38	0.59
1:C:246:ASP:O	1:C:247:ARG:CB	2.49	0.59
1:B:25:ASN:ND2	1:B:60:THR:CB	2.66	0.58
1:B:25:ASN:C	3:B:2006:HOH:O	2.24	0.58
1:C:240:ASP:CB	1:C:241:MET:CB	2.82	0.58
1:C:246:ASP:O	1:C:247:ARG:HB3	2.04	0.57
1:B:71:LEU:HD13	1:B:77:TRP:CB	2.34	0.57
1:C:47:PHE:HB2	1:C:130:MET:HE1	1.86	0.57
2:A:1260:PEG:O4	2:A:1261:PEG:C1	2.53	0.57
1:B:153:GLN:HB2	3:B:2033:HOH:O	2.01	0.57
1:C:240:ASP:HB2	1:C:241:MET:CB	2.27	0.57
1:C:142:ASP:OD1	1:C:143:TYR:N	2.38	0.57
1:C:119:ASP:O	1:C:123:GLU:HG2	2.05	0.56
1:C:133:ASP:OD1	1:C:135:VAL:HG22	2.05	0.56
1:D:119:ASP:O	1:D:123:GLU:HG2	2.05	0.56
1:A:34:ARG:O	1:A:38:LEU:HD13	2.05	0.56
1:C:71:LEU:HD13	1:C:77:TRP:HB3	1.85	0.56
1:B:138:GLU:HG2	3:B:2031:HOH:O	2.05	0.56
1:A:25:ASN:HD21	1:A:60:THR:HG22	1.65	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:NE2	3:A:2032:HOH:O	2.26	0.56
1:B:149:THR:HG23	1:B:150:PHE:CD2	2.41	0.56
1:C:148:LEU:O	1:C:149:THR:CB	2.53	0.56
1:C:194:CYS:SG	1:C:195:VAL:HG13	2.47	0.55
1:B:119:ASP:O	1:B:123:GLU:HG2	2.07	0.55
1:A:119:ASP:O	1:A:123:GLU:HG2	2.07	0.55
1:D:203:ILE:HD12	1:D:223:VAL:CG1	2.37	0.55
1:C:36:LEU:HA	1:C:39:LEU:HD12	1.89	0.55
1:C:154:ASP:HB3	1:C:245:MET:CE	2.36	0.55
1:B:148:LEU:C	1:B:149:THR:CG2	2.75	0.54
1:B:238:LEU:O	1:B:239:SER:HB3	2.06	0.54
1:D:127:HIS:ND1	1:D:182:GLY:HA3	2.22	0.54
1:A:157:LEU:HD23	1:A:245:MET:HG2	1.90	0.54
1:D:21:SER:O	1:D:22:ALA:C	2.45	0.54
1:D:236:PHE:CD2	1:D:237:VAL:HG13	2.43	0.54
1:A:148:LEU:C	1:A:150:PHE:N	2.58	0.54
1:B:228:ASP:OD2	1:C:172:LYS:NZ	2.36	0.54
1:A:75:THR:HG22	1:A:134:ARG:HD2	1.90	0.54
1:A:75:THR:HG22	1:A:134:ARG:CD	2.38	0.53
1:D:254:LEU:CD1	1:D:254:LEU:N	2.71	0.53
1:A:32:PHE:CD1	1:A:58:SER:HB2	2.44	0.53
1:B:25:ASN:ND2	1:B:60:THR:CG2	2.71	0.53
1:D:245:MET:O	1:D:248:ALA:HB3	2.09	0.53
1:B:127:HIS:HE1	1:B:167:GLU:OE2	1.92	0.52
1:B:148:LEU:N	1:B:148:LEU:HD12	2.25	0.52
1:B:32:PHE:CD1	1:B:58:SER:HB2	2.43	0.52
1:B:153:GLN:CG	3:B:2033:HOH:O	2.40	0.52
1:A:240:ASP:OD1	1:A:241:MET:O	2.27	0.52
1:A:205:PHE:CD2	1:A:227:ILE:HD11	2.45	0.52
1:D:34:ARG:O	1:D:38:LEU:HD13	2.10	0.52
1:B:133:ASP:OD1	1:B:135:VAL:HG22	2.09	0.52
1:D:228:ASP:H	1:D:232:ASN:ND2	2.08	0.52
1:D:240:ASP:OD1	1:D:241:MET:O	2.28	0.52
1:D:144:ALA:O	1:D:147:VAL:HG22	2.10	0.52
1:B:23:GLN:O	3:B:2006:HOH:O	2.19	0.51
1:D:35:GLN:NE2	1:D:188:ILE:HG22	2.25	0.51
1:B:148:LEU:HA	1:B:150:PHE:H	1.76	0.51
1:C:35:GLN:NE2	1:C:188:ILE:HG22	2.25	0.51
1:C:173:THR:HA	3:C:2016:HOH:O	2.10	0.51
1:D:233:LEU:O	1:D:236:PHE:O	2.28	0.51
1:A:47:PHE:CG	1:A:185:LEU:HD13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:C	1:A:241:MET:O	2.46	0.51
1:A:13:ASP:OD1	1:A:17:LEU:N	2.44	0.51
1:C:47:PHE:HB2	1:C:130:MET:CE	2.41	0.51
1:B:148:LEU:O	1:B:149:THR:CB	2.59	0.50
2:A:1261:PEG:C4	2:A:1262:PEG:HO4	2.24	0.50
2:B:1260:PEG:H32	3:B:2049:HOH:O	2.11	0.50
1:B:13:ASP:OD1	1:B:17:LEU:N	2.45	0.50
1:C:144:ALA:O	1:C:147:VAL:HG22	2.12	0.50
1:A:15:GLN:HG3	1:A:17:LEU:HD22	1.93	0.50
1:B:39:LEU:N	1:B:40:PRO:CD	2.75	0.50
1:B:34:ARG:O	1:B:38:LEU:HD13	2.11	0.50
1:C:32:PHE:CD1	1:C:58:SER:HB2	2.47	0.50
1:B:39:LEU:N	1:B:40:PRO:HD2	2.26	0.49
1:A:144:ALA:O	1:A:147:VAL:HG22	2.12	0.49
2:A:1261:PEG:H42	2:A:1262:PEG:O4	2.12	0.49
1:B:256:PRO:O	1:B:258:PHE:N	2.43	0.49
1:D:32:PHE:CD1	1:D:58:SER:HB2	2.47	0.49
1:A:25:ASN:ND2	1:A:60:THR:CG2	2.64	0.49
1:B:212:ARG:CZ	1:B:254:LEU:HD11	2.43	0.49
1:C:154:ASP:HB3	1:C:245:MET:HE3	1.94	0.49
1:D:26:ARG:O	1:D:30:ILE:HG22	2.12	0.49
1:D:254:LEU:N	1:D:254:LEU:HD12	2.28	0.49
1:A:227:ILE:HG13	1:A:232:ASN:HD22	1.78	0.48
1:D:212:ARG:NE	1:D:254:LEU:HD11	2.28	0.48
1:B:77:TRP:CD1	1:B:137:ALA:HB1	2.48	0.48
1:B:228:ASP:H	1:B:232:ASN:HD21	1.59	0.48
1:A:203:ILE:HD12	1:A:223:VAL:HG13	1.96	0.48
1:B:227:ILE:HG23	1:B:229:SER:H	1.79	0.48
2:A:1260:PEG:C2	2:A:1262:PEG:O4	2.61	0.48
1:A:205:PHE:CG	1:A:227:ILE:HD12	2.48	0.48
1:B:237:VAL:C	1:B:238:LEU:O	2.48	0.48
1:D:112:LEU:HD23	1:D:113:ASP:H	1.78	0.48
1:A:47:PHE:CD2	1:A:185:LEU:HD13	2.48	0.48
1:A:18:VAL:CG2	1:A:20:TYR:CZ	2.96	0.47
1:A:163:TRP:HE3	2:A:1262:PEG:HO1	1.59	0.47
1:C:139:PHE:O	1:C:142:ASP:OD1	2.32	0.47
1:A:57:ASN:CG	1:A:59:SER:HB3	2.34	0.47
1:A:146:LYS:O	1:A:150:PHE:HD2	1.98	0.47
1:B:177:LEU:HD21	1:B:202:ARG:HD3	1.95	0.47
1:D:205:PHE:CB	1:D:227:ILE:HD12	2.43	0.47
1:B:15:GLN:HG3	1:B:17:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:CYS:HG	1:C:130:MET:CE	2.20	0.47
1:A:216:ARG:HG2	1:A:258:PHE:CE1	2.49	0.47
1:C:216:ARG:HG2	1:C:258:PHE:CE1	2.49	0.47
1:B:203:ILE:HD12	1:B:223:VAL:HG13	1.96	0.47
1:A:247:ARG:CA	1:A:250[B]:GLU:HG2	2.41	0.47
1:C:35:GLN:HE22	1:C:188:ILE:CG2	2.28	0.47
1:B:53:THR:HG21	1:B:74:LYS:HG3	1.96	0.46
1:D:154:ASP:HB3	1:D:245:MET:CE	2.45	0.46
1:A:31:LEU:HD11	1:A:107:ARG:HD2	1.97	0.46
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.64	0.46
1:A:116:GLN:HE22	1:A:218:ASP:HB3	1.79	0.46
1:B:77:TRP:NE1	1:B:137:ALA:HB1	2.31	0.46
1:C:245:MET:O	1:C:248:ALA:HB3	2.16	0.46
1:D:148:LEU:O	1:D:149:THR:CB	2.63	0.46
2:B:1260:PEG:C3	3:B:2049:HOH:O	2.64	0.46
1:C:205:PHE:CD2	1:C:227:ILE:HD11	2.51	0.46
1:D:205:PHE:HB2	1:D:227:ILE:HD12	1.97	0.46
1:B:146:LYS:O	1:B:150:PHE:HD2	1.97	0.46
1:B:236:PHE:CD2	1:B:237:VAL:HG23	2.51	0.46
1:C:161:MET:HE3	1:C:161:MET:O	2.15	0.46
1:D:27:ILE:HA	1:D:30:ILE:HG23	1.97	0.46
1:A:163:TRP:HE3	2:A:1262:PEG:O1	2.00	0.45
1:D:205:PHE:CD2	1:D:227:ILE:HD11	2.51	0.45
1:A:39:LEU:N	1:A:40:PRO:HD2	2.31	0.45
2:A:1260:PEG:O4	2:A:1261:PEG:H12	2.16	0.45
1:C:77:TRP:CD1	1:C:137:ALA:HB1	2.52	0.45
1:D:82:VAL:O	1:D:103:ALA:HA	2.16	0.45
2:B:1260:PEG:O4	2:B:1261:PEG:H31	2.17	0.45
1:B:218:ASP:OD1	1:B:218:ASP:N	2.49	0.45
1:A:30:ILE:HD13	1:A:112:LEU:HD11	1.98	0.45
1:C:142:ASP:CG	1:C:237:VAL:CG1	2.70	0.45
1:C:237:VAL:C	1:C:238:LEU:O	2.48	0.45
1:D:39:LEU:N	1:D:40:PRO:HD2	2.32	0.45
1:D:146:LYS:O	1:D:150:PHE:HD2	2.00	0.45
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.82	0.45
1:B:227:ILE:HD13	1:B:233:LEU:HD21	1.99	0.45
1:B:251:LEU:HD21	1:C:199:ILE:HD11	1.99	0.44
1:D:216:ARG:HG2	1:D:258:PHE:CE1	2.51	0.44
1:C:146:LYS:O	1:C:150:PHE:HD2	1.99	0.44
1:A:19:ASP:CG	1:A:19:ASP:O	2.53	0.44
1:B:38:LEU:HD23	1:B:192:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:CZ	1:C:188:ILE:CD1	2.95	0.44
1:C:205:PHE:CG	1:C:227:ILE:HD12	2.53	0.44
1:A:18:VAL:CG2	1:A:18:VAL:O	2.66	0.43
1:B:25:ASN:HD22	1:B:60:THR:CG2	2.27	0.43
1:A:27:ILE:HA	1:A:30:ILE:HG23	2.00	0.43
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.63	0.43
1:B:248:ALA:O	1:B:251:LEU:O	2.36	0.43
1:C:34:ARG:O	1:C:38:LEU:HD13	2.17	0.43
1:D:195:VAL:O	1:D:195:VAL:HG23	2.17	0.43
1:C:35:GLN:NE2	1:C:188:ILE:CG2	2.81	0.43
1:A:39:LEU:N	1:A:40:PRO:CD	2.81	0.43
1:D:148:LEU:HD12	1:D:148:LEU:N	2.33	0.43
1:C:130:MET:HE3	1:C:180:TYR:CB	2.48	0.43
1:B:25:ASN:HD21	1:B:60:THR:HB	1.82	0.43
1:B:32:PHE:CE1	1:B:58:SER:HB2	2.54	0.43
1:A:38:LEU:HD23	1:A:192:VAL:HG23	2.01	0.42
1:A:74:LYS:O	1:A:134:ARG:HD3	2.19	0.42
1:A:135:VAL:CG2	1:A:230:TYR:HB2	2.49	0.42
1:C:227:ILE:HG13	1:C:232:ASN:HD22	1.84	0.42
1:D:35:GLN:HE22	1:D:188:ILE:CG2	2.31	0.42
1:D:35:GLN:HE22	1:D:188:ILE:HG22	1.83	0.42
1:B:251:LEU:HD21	1:C:199:ILE:CD1	2.50	0.42
1:A:205:PHE:CB	1:A:227:ILE:HD12	2.49	0.42
1:B:92:PHE:CG	1:B:147:VAL:HG21	2.54	0.42
1:C:195:VAL:HG23	1:C:196:GLU:HG3	2.01	0.42
1:D:39:LEU:N	1:D:40:PRO:CD	2.83	0.42
1:A:37:LYS:NZ	3:A:2007:HOH:O	1.90	0.42
1:A:71:LEU:HD13	1:A:77:TRP:HB3	2.00	0.42
1:A:161:MET:HB3	1:A:161:MET:HE2	1.59	0.42
1:D:100:PHE:HZ	1:D:127:HIS:HD2	1.68	0.42
1:A:34:ARG:CZ	1:A:188:ILE:CD1	2.97	0.42
1:A:213:MET:CE	1:D:257:TYR:OH	2.68	0.42
1:D:77:TRP:CD1	1:D:137:ALA:HB1	2.55	0.42
1:A:242:GLY:N	1:A:245:MET:HE2	2.33	0.42
1:D:31:LEU:HD11	1:D:107:ARG:CD	2.43	0.42
1:B:47:PHE:CG	1:B:185:LEU:HD13	2.54	0.41
1:C:39:LEU:N	1:C:40:PRO:HD2	2.35	0.41
1:C:114:TYR:HD1	1:C:114:TYR:H	1.68	0.41
1:D:234:TYR:CD1	1:D:238:LEU:HD11	2.55	0.41
1:A:25:ASN:ND2	1:A:60:THR:HA	2.35	0.41
1:C:71:LEU:HD13	1:C:77:TRP:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD22	1:B:62:PRO:CG	2.50	0.41
1:B:160:ARG:HD3	1:B:213:MET:O	2.21	0.41
1:D:185:LEU:HD23	1:D:185:LEU:HA	1.89	0.41
1:A:117:GLU:HA	1:A:118:PRO:HD2	1.89	0.41
1:D:240:ASP:C	1:D:241:MET:O	2.59	0.41
1:A:18:VAL:CG2	1:A:20:TYR:CE2	3.04	0.41
1:A:32:PHE:CE1	1:A:58:SER:HB2	2.56	0.41
1:A:240:ASP:CG	1:A:241:MET:O	2.59	0.41
1:D:25:ASN:ND2	1:D:60:THR:HA	2.36	0.41
1:A:218:ASP:N	1:A:218:ASP:OD1	2.52	0.41
1:C:163:TRP:CZ2	1:C:168:PHE:CE2	3.08	0.41
1:A:42:ARG:NE	1:A:196:GLU:OE2	2.54	0.41
1:A:57:ASN:HD21	1:A:59:SER:HB3	1.84	0.41
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.90	0.41
1:B:134:ARG:NH1	1:B:134:ARG:HG2	2.35	0.41
1:B:154:ASP:HB3	1:B:245:MET:HE3	2.02	0.41
1:D:38:LEU:HD23	1:D:192:VAL:CG2	2.50	0.41
1:A:53:THR:HG21	1:A:74:LYS:HG3	2.02	0.41
1:B:82:VAL:O	1:B:103:ALA:HA	2.21	0.41
1:A:77:TRP:CD1	1:A:137:ALA:HB1	2.56	0.41
1:B:56:LEU:HD22	1:B:62:PRO:HG2	2.03	0.41
1:A:38:LEU:HD23	1:A:192:VAL:CG2	2.51	0.40
1:A:155:TRP:N	1:A:156:PRO:CD	2.84	0.40
1:C:160:ARG:HD3	1:C:213:MET:O	2.22	0.40
1:B:47:PHE:CD2	1:B:185:LEU:HD13	2.56	0.40
1:C:172:LYS:HD3	1:C:177:LEU:HD13	2.04	0.40
1:D:219:GLN:HE22	1:D:258:PHE:CB	2.35	0.40
1:B:134:ARG:HG2	1:B:134:ARG:HH11	1.86	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	251/272 (92%)	227 (90%)	20 (8%)	4 (2%)	9 17
1	B	250/272 (92%)	223 (89%)	21 (8%)	6 (2%)	6 9
1	C	230/272 (85%)	203 (88%)	21 (9%)	6 (3%)	5 8
1	D	233/272 (86%)	206 (88%)	17 (7%)	10 (4%)	2 3
All	All	964/1088 (89%)	859 (89%)	79 (8%)	26 (3%)	5 7

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	MET
1	A	247	ARG
1	B	22	ALA
1	B	247	ARG
1	C	84	ALA
1	C	247	ARG
1	D	22	ALA
1	D	83	ALA
1	D	237	VAL
1	D	247	ARG
1	A	152	GLU
1	B	149	THR
1	B	257	TYR
1	C	149	THR
1	C	152	GLU
1	C	241	MET
1	D	24	GLU
1	D	149	THR
1	D	152	GLU
1	D	240	ASP
1	B	152	GLU
1	B	219	GLN
1	C	219	GLN
1	D	219	GLN
1	D	241	MET
1	A	219	GLN

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	223/241 (92%)	195 (87%)	28 (13%)	4 8
1	B	222/241 (92%)	195 (88%)	27 (12%)	5 9
1	C	206/241 (86%)	178 (86%)	28 (14%)	3 7
1	D	210/241 (87%)	184 (88%)	26 (12%)	4 9
All	All	861/964 (89%)	752 (87%)	109 (13%)	4 8

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	18	VAL
1	A	21	SER
1	A	30	ILE
1	A	33	GLU
1	A	40	PRO
1	A	48	LEU
1	A	51	LEU
1	A	68	SER
1	A	71	LEU
1	A	89	ARG
1	A	98	LYS
1	A	116	GLN
1	A	139	PHE
1	A	152	GLU
1	A	157	LEU
1	A	161	MET
1	A	188	ILE
1	A	213	MET
1	A	216	ARG
1	A	227	ILE
1	A	239	SER
1	A	243	LYS
1	A	245	MET
1	A	246	ASP
1	A	250[A]	GLU
1	A	250[B]	GLU
1	A	259	ASP
1	B	11	VAL
1	B	17	LEU

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Mol	Chain	Res	Type
1	B	21	SER
1	B	30	ILE
1	B	33	GLU
1	B	40	PRO
1	B	48	LEU
1	B	51	LEU
1	B	68	SER
1	B	71	LEU
1	B	72	LYS
1	B	89	ARG
1	B	98	LYS
1	B	116	GLN
1	B	148	LEU
1	B	152	GLU
1	B	157	LEU
1	B	161	MET
1	B	188	ILE
1	B	195	VAL
1	B	196	GLU
1	B	213	MET
1	B	227	ILE
1	B	239	SER
1	B	243	LYS
1	B	246	ASP
1	B	249	ARG
1	C	30	ILE
1	C	33	GLU
1	C	40	PRO
1	C	48	LEU
1	C	51	LEU
1	C	68	SER
1	C	71	LEU
1	C	85	LEU
1	C	98	LYS
1	C	114	TYR
1	C	116	GLN
1	C	117	GLU
1	C	149	THR
1	C	152	GLU
1	C	153	GLN
1	C	157	LEU
1	C	159	GLN

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Mol	Chain	Res	Type
1	C	161	MET
1	C	188	ILE
1	C	207	PRO
1	C	216	ARG
1	C	227	ILE
1	C	234	TYR
1	C	235	ASP
1	C	237	VAL
1	C	243	LYS
1	C	250	GLU
1	C	259	ASP
1	D	21	SER
1	D	30	ILE
1	D	33	GLU
1	D	40	PRO
1	D	48	LEU
1	D	51	LEU
1	D	68	SER
1	D	71	LEU
1	D	72	LYS
1	D	85	LEU
1	D	89	ARG
1	D	110	GLU
1	D	131	LEU
1	D	148	LEU
1	D	152	GLU
1	D	157	LEU
1	D	161	MET
1	D	172	LYS
1	D	188	ILE
1	D	196	GLU
1	D	216	ARG
1	D	227	ILE
1	D	234	TYR
1	D	241	MET
1	D	243	LYS
1	D	246	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN

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Mol	Chain	Res	Type
1	A	35	GLN
1	A	57	ASN
1	A	116	GLN
1	A	219	GLN
1	A	232	ASN
1	B	25	ASN
1	B	35	GLN
1	B	232	ASN
1	C	35	GLN
1	C	232	ASN
1	D	25	ASN
1	D	35	GLN
1	D	219	GLN
1	D	232	ASN

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)

6 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	PEG	B	1260	-	6,6,6	1.01	0	5,5,5	0.73	0
2	PEG	A	1260	-	6,6,6	0.76	0	5,5,5	1.01	0
2	PEG	A	1262	-	6,6,6	1.42	2 (33%)	5,5,5	0.61	0
2	PEG	A	1261	-	6,6,6	0.66	0	5,5,5	0.55	0
2	PEG	B	1262	-	6,6,6	0.74	0	5,5,5	1.31	1 (20%)
2	PEG	B	1261	-	6,6,6	0.46	0	5,5,5	0.90	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	PEG	B	1260	-	-	4/4/4/4	-
2	PEG	A	1260	-	-	3/4/4/4	-
2	PEG	A	1262	-	-	3/4/4/4	-
2	PEG	A	1261	-	-	3/4/4/4	-
2	PEG	B	1262	-	-	3/4/4/4	-
2	PEG	B	1261	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1262	PEG	C3-C4	2.55	1.63	1.49
2	A	1262	PEG	O2-C3	2.21	1.51	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1262	PEG	C3-O2-C2	2.19	122.79	113.29

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1260	PEG	C4-C3-O2-C2
2	B	1262	PEG	C4-C3-O2-C2
2	A	1262	PEG	C4-C3-O2-C2
2	B	1262	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	B	1260	PEG	C1-C2-O2-C3
2	A	1260	PEG	O2-C3-C4-O4
2	A	1262	PEG	O2-C3-C4-O4
2	A	1260	PEG	C4-C3-O2-C2
2	A	1261	PEG	O1-C1-C2-O2
2	A	1262	PEG	O1-C1-C2-O2
2	B	1260	PEG	O1-C1-C2-O2
2	B	1260	PEG	O2-C3-C4-O4
2	A	1260	PEG	O1-C1-C2-O2
2	B	1261	PEG	C4-C3-O2-C2
2	B	1261	PEG	C1-C2-O2-C3
2	B	1262	PEG	C1-C2-O2-C3
2	A	1261	PEG	C1-C2-O2-C3
2	B	1261	PEG	O2-C3-C4-O4
2	A	1261	PEG	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1260	PEG	8	0
2	A	1260	PEG	4	0
2	A	1262	PEG	10	0
2	A	1261	PEG	8	0
2	B	1262	PEG	1	0
2	B	1261	PEG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	108:SER	C	109:GLU	N	1.75
1	D	82:VAL	C	83:ALA	N	1.66
1	D	83:ALA	C	84:ALA	N	1.17
1	C	81:PRO	C	82:VAL	N	0.74
1	C	109:GLU	C	110:GLU	N	0.67

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	252/272 (92%)	-0.24	1 (0%)	92	93	15, 27, 49, 84	4 (1%)
1	B	252/272 (92%)	-0.22	1 (0%)	92	93	16, 29, 56, 90	5 (1%)
1	C	229/272 (84%)	0.97	46 (20%)	1	0	19, 65, 111, 130	56 (24%)
1	D	235/272 (86%)	0.91	42 (17%)	1	1	21, 64, 93, 115	40 (17%)
All	All	968/1088 (88%)	0.33	90 (9%)	8	8	15, 40, 92, 130	105 (10%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	GLN	11.4
1	C	99	TYR	9.5
1	C	113	ASP	7.0
1	C	114	TYR	6.7
1	D	114	TYR	6.7
1	D	103	ALA	6.0
1	C	91	PHE	5.8
1	D	110	GLU	5.5
1	D	112	LEU	5.3
1	C	117	GLU	5.3
1	C	149	THR	5.3
1	C	100	PHE	5.3
1	D	104	THR	5.1
1	D	238	LEU	5.0
1	D	108	SER	4.8
1	C	103	ALA	4.7
1	C	60	THR	4.6
1	D	99	TYR	4.5
1	C	216	ARG	4.4
1	D	102	ALA	4.2
1	D	93	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	128	CYS	4.1
1	D	113	ASP	4.1
1	C	32	PHE	4.0
1	C	33	GLU	3.9
1	D	22	ALA	3.8
1	D	175	LYS	3.8
1	D	86	ILE	3.7
1	D	109	GLU	3.7
1	C	84	ALA	3.7
1	C	234	TYR	3.6
1	D	61	ILE	3.5
1	C	104	THR	3.5
1	D	94	LEU	3.5
1	D	54	LEU	3.3
1	C	147	VAL	3.2
1	C	28	TRP	3.1
1	C	56	LEU	3.1
1	C	115	VAL	3.1
1	C	110	GLU	3.1
1	D	82	VAL	3.0
1	C	118	PRO	3.0
1	C	51	LEU	3.0
1	C	71	LEU	3.0
1	D	95	LEU	3.0
1	C	111	GLU	3.0
1	C	148	LEU	3.0
1	D	59	SER	3.0
1	D	71	LEU	2.9
1	C	123	GLU	2.9
1	C	153	GLN	2.9
1	C	108	SER	2.8
1	D	56	LEU	2.8
1	D	28	TRP	2.8
1	C	124	LEU	2.8
1	D	148	LEU	2.7
1	D	77	TRP	2.7
1	D	100	PHE	2.7
1	D	98	LYS	2.7
1	D	162	PHE	2.7
1	C	217	ILE	2.7
1	D	63	GLN	2.7
1	D	60	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	124	LEU	2.6
1	B	259	ASP	2.6
1	C	31	LEU	2.4
1	C	75	THR	2.4
1	D	79	VAL	2.4
1	A	114	TYR	2.4
1	C	57	ASN	2.4
1	D	105	PHE	2.3
1	C	154	ASP	2.3
1	D	65	PRO	2.3
1	D	131	LEU	2.3
1	D	237	VAL	2.3
1	C	79	VAL	2.2
1	D	147	VAL	2.2
1	C	102	ALA	2.2
1	C	65	PRO	2.2
1	C	143	TYR	2.2
1	C	130	MET	2.2
1	C	150	PHE	2.2
1	D	32	PHE	2.2
1	C	105	PHE	2.2
1	C	142	ASP	2.2
1	C	258	PHE	2.1
1	C	30	ILE	2.1
1	D	85	LEU	2.1
1	D	101	PRO	2.1
1	D	57	ASN	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	PEG	A	1262	7/7	0.89	0.17	13,23,27,33	0
2	PEG	A	1261	7/7	0.92	0.15	27,29,34,36	0
2	PEG	B	1262	7/7	0.93	0.13	36,39,46,47	0
2	PEG	A	1260	7/7	0.96	0.12	12,14,17,20	0
2	PEG	B	1261	7/7	0.97	0.11	24,28,34,36	0
2	PEG	B	1260	7/7	0.98	0.09	12,12,14,15	0

6.5 Other polymers (i)

There are no such residues in this entry.