Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:43 PM GMT

PDB ID	:	1LOA
Title	:	THREE-DIMENSIONAL STRUCTURES OF COMPLEXES OF LATHYRUS OCHRUS ISOLECTIN I WITH GLUCOSE AND MANNOSE: FINE SPECIFICITY OF THE MONOSACCHARIDE-BINDING SITE
Authors	:	Bourne, Y.; Cambillau, C.
Deposited on	:	1993-01-27
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

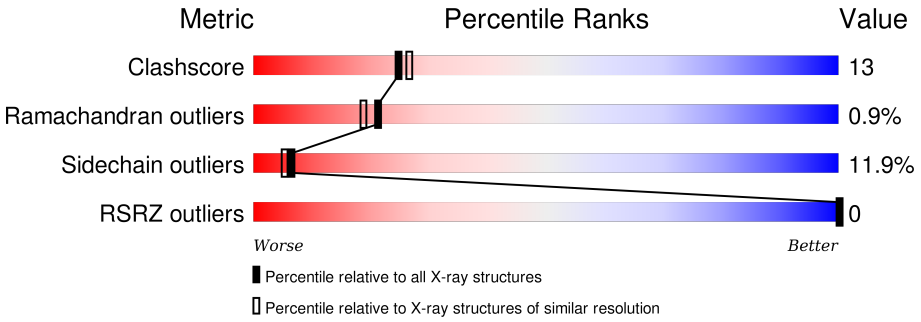
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	181	62% 31% 6% •
1	C	181	64% 28% 8% ••
1	E	181	60% 30% 5% • •
1	G	181	59% 33% 7% ••
2	B	52	67% 23% 10%
2	D	52	65% 19% 6% 10%
2	F	52	50% 37% • 10%

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Mol	Chain	Length	Quality of chain
2	H	52	

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
4	CA	C	458	-	-	-	X
5	MN	F	689	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7460 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 LEGUME ISOLECTIN I (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	C	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	E	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	G	180	Total	C	N	O	0	0	0
			1397	890	230	277			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	LYS	CONFLICT	UNP P04122
C	153	ALA	LYS	CONFLICT	UNP P04122
E	153	ALA	LYS	CONFLICT	UNP P04122
G	153	ALA	LYS	CONFLICT	UNP P04122

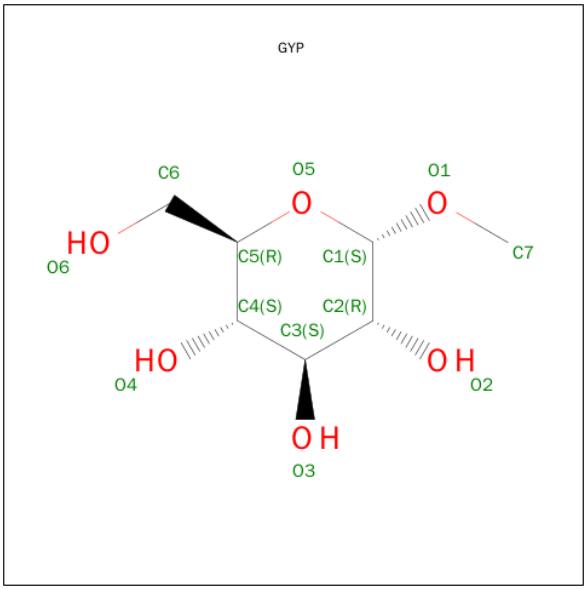
- Molecule 2 is a protein called LEGUME ISOLECTIN I (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	D	47	Total	C	N	O	0	0	0
			376	248	58	70			
2	F	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	H	47	Total	C	N	O	0	0	0
			376	248	58	70			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	TYR	PHE	CONFLICT	UNP P12306
D	41	TYR	PHE	CONFLICT	UNP P12306
F	41	TYR	PHE	CONFLICT	UNP P12306
H	41	TYR	PHE	CONFLICT	UNP P12306

- Molecule 3 is SUGAR (O1-METHYL-GLUCOSE) (three-letter code: GYP) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 7 6	0	0
3	C	1	Total C O 13 7 6	0	0
3	E	1	Total C O 13 7 6	0	0
3	G	1	Total C O 13 7 6	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Ca 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Mn 1 1	0	0
5	A	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0
5	F	1	Total Mn 1 1	0	0

- Molecule 6 is water.

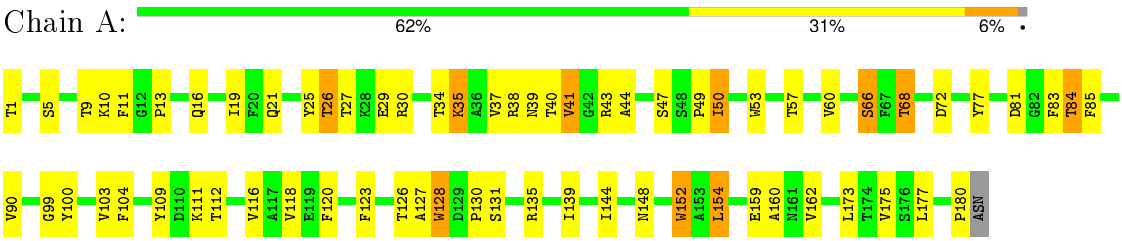
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	73	Total O 73 73	0	0
6	B	17	Total O 17 17	0	0
6	C	59	Total O 59 59	0	0
6	D	8	Total O 8 8	0	0
6	E	53	Total O 53 53	0	0
6	F	9	Total O 9 9	0	0
6	G	70	Total O 70 70	0	0
6	H	9	Total O 9 9	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

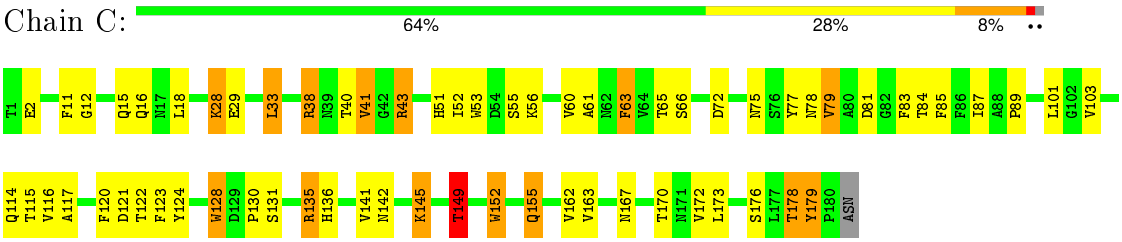
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain A:



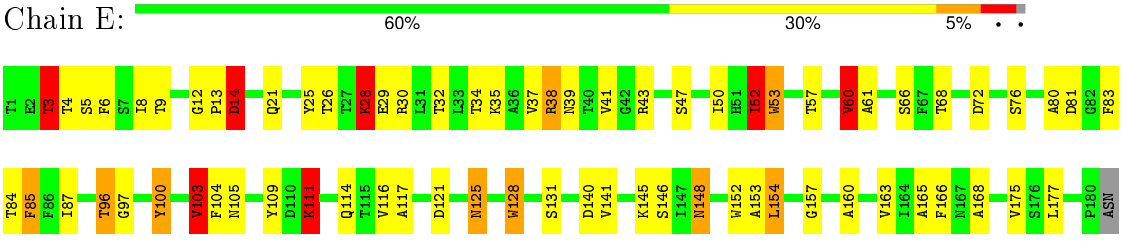
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain C:



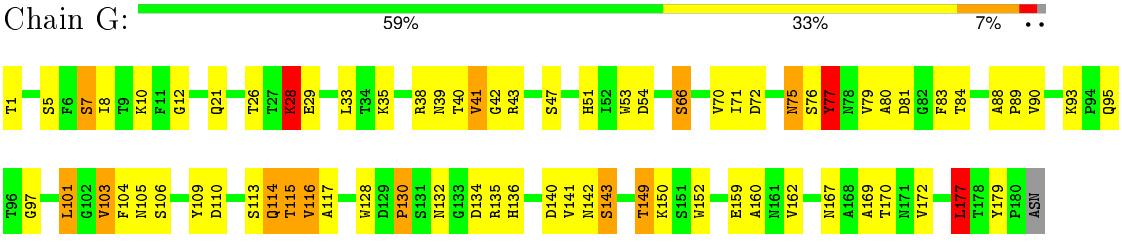
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain E:



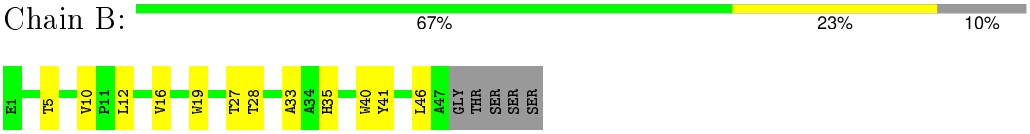
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain G:



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain B:

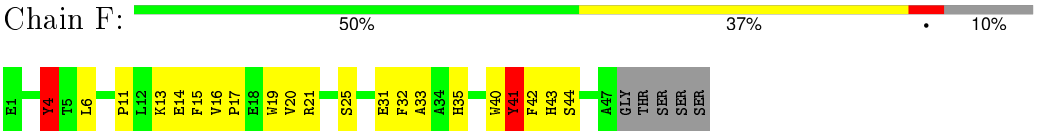


• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain D:

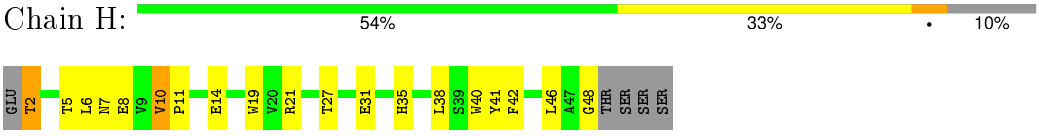
• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain F:



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

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	56.30Å 139.80Å 62.70Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 7.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.20) 67.2 (7.99-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 71.6	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 32074 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7460	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, GYP

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	1.04	0/1431	1.82	34/1954 (1.7%)
1	C	0.96	0/1431	1.83	30/1954 (1.5%)
1	E	1.01	1/1431 (0.1%)	1.85	32/1954 (1.6%)
1	G	0.99	1/1431 (0.1%)	1.76	18/1954 (0.9%)
2	B	1.17	0/394	1.75	7/539 (1.3%)
2	D	1.03	0/389	1.84	9/532 (1.7%)
2	F	1.13	0/394	1.91	9/539 (1.7%)
2	H	1.17	0/389	1.81	9/532 (1.7%)
All	All	1.03	2/7290 (0.0%)	1.82	148/9958 (1.5%)

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	E	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	116	VAL	CA-CB	6.01	1.67	1.54
1	E	60	VAL	CA-CB	5.81	1.67	1.54

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	4	TYR	CB-CG-CD1	-13.97	112.62	121.00
2	H	41	TYR	CB-CG-CD1	-10.87	114.48	121.00
1	E	152	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	C	172	VAL	CG1-CB-CG2	-9.20	96.18	110.90
1	E	100	TYR	CB-CG-CD1	-9.06	115.56	121.00
1	C	124	TYR	CB-CG-CD2	-8.95	115.63	121.00
1	A	152	TRP	CD1-CG-CD2	8.59	113.17	106.30
1	G	172	VAL	CG1-CB-CG2	-8.38	97.50	110.90
2	F	21	ARG	NE-CZ-NH1	8.31	124.45	120.30
2	H	19	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	E	175	VAL	CG1-CB-CG2	-8.06	98.01	110.90
1	A	135	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	E	109	TYR	CB-CG-CD2	-8.03	116.18	121.00
1	E	128	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	G	128	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	E	152	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	C	152	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	A	128	TRP	CG-CD2-CE3	7.92	141.03	133.90
2	D	21	ARG	NE-CZ-NH2	-7.91	116.34	120.30
2	D	19	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	G	38	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	C	53	TRP	CA-CB-CG	7.65	128.24	113.70
1	G	152	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	123	PHE	CA-C-N	-7.57	100.54	117.20
1	C	135	ARG	NE-CZ-NH2	-7.49	116.56	120.30
2	D	37	VAL	CA-CB-CG2	-7.42	99.77	110.90
1	C	53	TRP	CD1-CG-CD2	7.42	112.23	106.30
1	A	128	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	G	77	TYR	CB-CG-CD1	-7.31	116.61	121.00
2	D	40	TRP	CE2-CD2-CG	-7.28	101.48	107.30
1	E	177	LEU	CA-CB-CG	7.24	131.95	115.30
1	G	152	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	G	177	LEU	CA-CB-CG	7.23	131.92	115.30
1	C	38	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	G	28	LYS	CA-C-N	-7.17	101.42	117.20
1	G	135	ARG	NE-CZ-NH1	7.16	123.88	120.30
2	B	19	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	A	152	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	G	128	TRP	CD1-CG-CD2	7.07	111.95	106.30
1	E	128	TRP	CE2-CD2-CG	-7.04	101.67	107.30
2	B	40	TRP	CD1-CG-CD2	7.03	111.93	106.30
2	D	19	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	G	109	TYR	CB-CG-CD1	-6.96	116.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	LEU	CA-CB-CG	6.84	131.03	115.30
1	C	53	TRP	CE2-CD2-CG	-6.84	101.83	107.30
2	H	19	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	E	53	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	C	120	PHE	N-CA-C	-6.76	92.75	111.00
1	A	26	THR	N-CA-CB	-6.75	97.47	110.30
1	C	128	TRP	CE2-CD2-CG	-6.73	101.91	107.30
1	A	72	ASP	CB-CG-OD1	6.72	124.35	118.30
1	G	53	TRP	CD1-CG-CD2	6.72	111.68	106.30
2	H	40	TRP	CD1-CG-CD2	6.71	111.67	106.30
1	C	152	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	C	77	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	C	179	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	E	14	ASP	CA-CB-CG	6.68	128.09	113.40
1	E	53	TRP	CE2-CD2-CG	-6.63	102.00	107.30
2	D	40	TRP	CD1-CG-CD2	6.57	111.56	106.30
1	C	135	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	E	154	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	72	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	E	152	TRP	CG-CD1-NE1	-6.51	103.58	110.10
1	G	135	ARG	NE-CZ-NH2	-6.51	117.04	120.30
2	B	19	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	A	53	TRP	CD1-CG-CD2	6.49	111.49	106.30
1	A	38	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	G	53	TRP	CE2-CD2-CG	-6.33	102.23	107.30
1	E	41	VAL	CB-CA-C	-6.30	99.43	111.40
1	E	153	ALA	N-CA-C	-6.29	94.00	111.00
1	A	9	THR	N-CA-CB	-6.21	98.49	110.30
1	C	128	TRP	CD1-CG-CD2	6.21	111.27	106.30
2	B	40	TRP	CE2-CD2-CG	-6.19	102.35	107.30
2	H	40	TRP	CE2-CD2-CG	-6.18	102.35	107.30
1	C	152	TRP	CG-CD1-NE1	-6.17	103.93	110.10
1	E	103	VAL	CG1-CB-CG2	-6.17	101.03	110.90
1	A	53	TRP	CE2-CD2-CG	-6.10	102.42	107.30
2	B	41	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	A	128	TRP	NE1-CE2-CZ2	-6.08	123.72	130.40
2	H	41	TYR	CB-CG-CD2	6.02	124.61	121.00
1	A	84	THR	CA-CB-CG2	6.00	120.79	112.40
1	C	43	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	83	PHE	O-C-N	-5.98	113.13	122.70
1	A	128	TRP	CD1-CG-CD2	5.98	111.08	106.30
2	F	41	TYR	CB-CG-CD2	-5.97	117.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	TRP	CA-CB-CG	5.97	125.04	113.70
1	G	83	PHE	N-CA-CB	-5.93	99.92	110.60
1	E	152	TRP	CG-CD2-CE3	5.88	139.19	133.90
1	C	173	LEU	CA-CB-CG	5.85	128.76	115.30
2	F	40	TRP	CA-CB-CG	5.84	124.79	113.70
1	C	155	GLN	CA-C-N	-5.80	104.44	117.20
2	F	4	TYR	CZ-CE2-CD2	-5.80	114.58	119.80
1	A	50	ILE	CB-CG1-CD1	-5.74	97.83	113.90
1	A	112	THR	CA-CB-CG2	5.72	120.41	112.40
1	E	8	ILE	N-CA-C	-5.71	95.58	111.00
2	F	19	TRP	CE2-CD2-CG	-5.69	102.75	107.30
1	E	165	ALA	CB-CA-C	-5.68	101.58	110.10
1	A	120	PHE	N-CA-C	-5.66	95.71	111.00
1	E	3	THR	N-CA-CB	-5.65	99.57	110.30
1	C	53	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	E	85	PHE	N-CA-C	-5.62	95.81	111.00
1	E	87	ILE	N-CA-C	-5.62	95.84	111.00
1	C	83	PHE	CA-C-N	5.57	129.46	117.20
2	F	13	LYS	CB-CA-C	-5.57	99.26	110.40
1	A	123	PHE	O-C-N	5.56	131.60	122.70
1	A	152	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	85	PHE	N-CA-C	-5.51	96.11	111.00
1	E	125	ASN	N-CA-C	-5.50	96.14	111.00
1	A	109	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	C	63	PHE	CA-CB-CG	5.49	127.08	113.90
2	D	37	VAL	CA-CB-CG1	5.49	119.13	110.90
2	B	16	VAL	N-CA-CB	-5.46	99.49	111.50
2	H	2	THR	N-CA-CB	-5.45	99.94	110.30
1	E	160	ALA	CA-C-N	5.43	129.16	117.20
2	F	4	TYR	CD1-CG-CD2	5.41	123.85	117.90
1	C	149	THR	N-CA-CB	-5.39	100.05	110.30
2	H	19	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	154	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	55	SER	CA-C-N	5.31	128.88	117.20
1	E	39	ASN	N-CA-C	5.30	125.32	111.00
1	E	111	LYS	CA-CB-CG	5.27	124.99	113.40
1	E	121	ASP	N-CA-CB	-5.27	101.12	110.60
2	D	19	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	C	121	ASP	N-CA-CB	-5.25	101.16	110.60
2	F	19	TRP	CD1-CG-CD2	5.24	110.49	106.30
1	A	77	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	180	PRO	N-CA-C	5.21	125.64	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	VAL	CA-CB-CG2	-5.19	103.12	110.90
1	G	103	VAL	N-CA-CB	-5.19	100.08	111.50
1	A	84	THR	CA-CB-OG1	-5.19	98.11	109.00
1	A	128	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	E	4	THR	CA-CB-OG1	-5.14	98.21	109.00
1	E	47	SER	CA-C-N	5.11	128.44	117.20
1	A	118	VAL	N-CA-C	-5.11	97.22	111.00
1	E	30	ARG	N-CA-C	5.10	124.76	111.00
1	G	101	LEU	O-C-N	-5.08	114.56	123.20
2	D	19	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	C	85	PHE	N-CA-C	-5.06	97.34	111.00
1	C	85	PHE	CA-C-N	5.04	128.30	117.20
1	A	41	VAL	CA-CB-CG2	-5.04	103.34	110.90
1	C	83	PHE	N-CA-CB	-5.03	101.54	110.60
1	G	128	TRP	NE1-CE2-CD2	5.03	112.33	107.30
2	H	40	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	E	52	ILE	O-C-N	-5.02	114.67	122.70
1	A	116	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	E	157	GLY	CA-C-N	5.01	128.21	117.20
2	B	40	TRP	CG-CD1-NE1	-5.00	105.10	110.10
1	C	103	VAL	N-CA-CB	-5.00	100.49	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	41	TYR	Sidechain
1	E	25	TYR	Sidechain
2	F	4	TYR	Sidechain

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	1397	0	1346	29	0
1	C	1397	0	1346	29	0
1	E	1397	0	1346	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1397	0	1346	40	0
2	B	381	0	357	6	0
2	D	376	0	351	8	0
2	F	381	0	357	21	0
2	H	376	0	351	20	0
3	A	13	0	14	0	0
3	C	13	0	14	3	0
3	E	13	0	14	1	0
3	G	13	0	14	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	1	0
5	G	1	0	0	0	0
6	A	73	0	0	2	0
6	B	17	0	0	2	0
6	C	59	0	0	3	0
6	D	8	0	0	0	0
6	E	53	0	0	2	0
6	F	9	0	0	0	0
6	G	70	0	0	2	0
6	H	9	0	0	0	0
All	All	7460	0	6856	160	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 13.

All (160) 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:130:PRO:HG3	1:C:149:THR:HG21	1.51	0.92
1:E:84:THR:HG21	1:E:117:ALA:HB1	1.57	0.83
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.31	0.75
1:A:10:LYS:HD2	1:A:29:GLU:HB3	1.73	0.70
1:C:122:THR:HA	1:C:135:ARG:HG2	1.75	0.69
1:A:11:PHE:O	1:A:29:GLU:HA	1.93	0.68
1:E:21:GLN:NE2	1:E:43:ARG:HE	1.93	0.67
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LYS:HE2	1:E:28:LYS:O	1.95	0.67
1:C:114:GLN:HA	1:C:142:ASN:HD21	1.64	0.63
1:G:160:ALA:HB1	1:G:177:LEU:HD13	1.82	0.62
1:G:70:VAL:HG23	2:H:38:LEU:HD11	1.80	0.62
1:E:6:PHE:CE1	2:F:42:PHE:HB3	2.35	0.62
1:E:21:GLN:HE21	1:E:43:ARG:HE	1.46	0.61
1:E:116:VAL:HG12	1:E:141:VAL:HG23	1.81	0.61
1:A:83:PHE:HB2	6:B:69:HOH:O	2.00	0.61
1:G:89:PRO:HD3	1:G:114:GLN:O	2.01	0.61
1:E:96:THR:HG1	1:E:105:ASN:HA	1.66	0.60
1:E:128:TRP:HB2	1:E:145:LYS:HG3	1.84	0.60
1:G:75:ASN:H	1:G:75:ASN:HD22	1.50	0.59
1:E:38:ARG:HD3	2:F:32:PHE:CE1	2.36	0.59
1:C:63:PHE:CZ	1:C:87:ILE:HD11	2.37	0.59
1:E:148:ASN:ND2	2:F:6:LEU:HD11	2.18	0.58
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.52	0.58
1:E:96:THR:OG1	1:E:105:ASN:HA	2.03	0.58
1:E:97:GLY:O	1:E:100:TYR:HB2	2.04	0.57
1:E:84:THR:CG2	1:E:117:ALA:HB1	2.31	0.57
1:G:150:LYS:HB2	2:H:6:LEU:HD13	1.87	0.57
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.02	0.56
2:H:38:LEU:N	2:H:38:LEU:HD12	2.20	0.56
1:G:150:LYS:HE3	2:H:5:THR:O	2.05	0.56
1:G:90:VAL:HA	2:H:21:ARG:HG3	1.88	0.56
1:E:84:THR:HG22	1:E:85:PHE:N	2.20	0.56
1:C:63:PHE:HZ	1:C:87:ILE:HD11	1.70	0.55
1:C:128:TRP:HB2	1:C:145:LYS:HG2	1.89	0.55
1:E:13:PRO:HA	1:E:26:THR:HG23	1.88	0.55
1:G:71:ILE:HG12	2:H:35:HIS:HD2	1.72	0.55
1:C:12:GLY:HA3	6:C:489:HOH:O	2.08	0.54
1:G:167:ASN:HD21	1:G:169:ALA:HB3	1.72	0.54
2:H:11:PRO:HB2	2:H:14:GLU:HG2	1.89	0.54
1:E:148:ASN:CG	2:F:6:LEU:HD11	2.29	0.53
1:G:33:LEU:O	1:G:42:GLY:HA3	2.08	0.53
1:G:80:ALA:HB3	2:H:31:GLU:HB2	1.91	0.52
1:C:75:ASN:OD1	1:C:78:ASN:HB2	2.09	0.52
1:C:78:ASN:HB3	6:C:512:HOH:O	2.09	0.52
1:G:84:THR:HG23	1:G:117:ALA:HB1	1.91	0.52
1:A:41:VAL:HG22	2:B:27:THR:HG22	1.92	0.52
1:E:5:SER:OG	2:F:43:HIS:HD2	1.93	0.52
1:G:75:ASN:HD22	1:G:75:ASN:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:GLN:HB3	1:G:105:ASN:OD1	2.10	0.52
1:E:21:GLN:HE22	1:E:43:ARG:NH2	2.07	0.51
1:E:21:GLN:NE2	1:E:43:ARG:NE	2.59	0.51
2:F:11:PRO:HD2	2:F:15:PHE:CE2	2.46	0.51
1:E:114:GLN:HA	2:F:15:PHE:O	2.10	0.51
1:E:66:SER:OG	2:F:41:TYR:HD2	1.93	0.51
1:C:136:HIS:HA	1:C:152:TRP:HB3	1.93	0.51
1:A:100:TYR:HB3	1:A:104:PHE:O	2.11	0.51
1:A:25:TYR:CE2	1:A:27:THR:HB	2.46	0.51
1:C:38:ARG:O	1:C:40:THR:HG23	2.10	0.51
1:C:11:PHE:O	1:C:29:GLU:HA	2.10	0.51
1:A:1:THR:HA	2:B:46:LEU:O	2.10	0.51
2:H:38:LEU:HD12	2:H:38:LEU:H	1.74	0.51
1:E:114:GLN:HB3	2:F:17:PRO:HD3	1.92	0.51
1:G:77:TYR:CD1	1:G:77:TYR:N	2.79	0.51
1:C:60:VAL:HG12	1:C:61:ALA:H	1.75	0.50
1:A:21:GLN:HE22	1:A:43:ARG:NH2	2.06	0.50
2:F:11:PRO:HD2	2:F:15:PHE:HE2	1.76	0.50
1:A:16:GLN:HB2	2:D:19:TRP:CD2	2.47	0.50
1:E:66:SER:HG	2:F:41:TYR:HD2	1.59	0.49
1:A:127:ALA:HB3	1:A:128:TRP:CE3	2.48	0.49
1:A:66:SER:HA	1:A:162:VAL:O	2.13	0.49
1:G:1:THR:HA	2:H:46:LEU:O	2.13	0.49
1:A:10:LYS:HD3	6:B:64:HOH:O	2.14	0.48
1:G:21:GLN:HB2	1:G:43:ARG:HB2	1.95	0.48
1:C:2:GLU:OE1	1:C:51:HIS:HD2	1.95	0.48
1:A:13:PRO:HA	1:A:26:THR:HG23	1.96	0.48
1:E:14:ASP:HA	6:E:723:HOH:O	2.14	0.48
1:G:103:VAL:HG13	1:G:104:PHE:CD2	2.49	0.48
1:G:130:PRO:HG3	1:G:149:THR:HG21	1.97	0.47
1:G:5:SER:HA	2:H:42:PHE:O	2.14	0.47
1:G:75:ASN:H	1:G:75:ASN:ND2	2.12	0.47
1:C:41:VAL:HB	2:D:27:THR:HG22	1.97	0.47
1:E:83:PHE:HA	2:F:25:SER:O	2.14	0.47
1:E:105:ASN:HB2	6:E:697:HOH:O	2.14	0.47
1:A:139:ILE:HD13	1:A:173:LEU:HD23	1.96	0.47
1:E:103:VAL:HG12	1:E:104:PHE:CD2	2.49	0.47
1:G:41:VAL:HB	2:H:27:THR:HG22	1.96	0.47
1:C:66:SER:HB3	1:C:163:VAL:HG22	1.96	0.46
2:F:42:PHE:HE2	2:F:44:SER:HG	1.59	0.46
1:A:40:THR:HG22	1:A:41:VAL:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:GYP:H5	3:C:182:GYP:H7C3	1.96	0.46
1:E:80:ALA:CB	2:F:31:GLU:HB2	2.46	0.46
1:E:61:ALA:O	1:E:168:ALA:HB2	2.15	0.46
1:G:66:SER:HA	1:G:162:VAL:O	2.16	0.46
6:G:963:HOH:O	2:H:48:GLY:HA3	2.15	0.45
1:G:110:ASP:O	1:G:142:ASN:HB3	2.16	0.45
1:A:40:THR:HG22	1:A:41:VAL:H	1.81	0.45
2:H:7:ASN:O	2:H:8:GLU:HG2	2.17	0.45
6:C:509:HOH:O	2:D:21:ARG:HA	2.17	0.45
1:A:159:GLU:HG3	6:A:285:HOH:O	2.16	0.45
1:E:3:THR:HB	1:G:7:SER:OG	2.17	0.45
1:G:167:ASN:HD22	1:G:170:THR:H	1.65	0.45
1:C:84:THR:CG2	1:C:117:ALA:HB1	2.47	0.45
1:C:61:ALA:HB1	2:D:45:GLU:O	2.17	0.45
1:E:166:PHE:CE2	1:E:168:ALA:HA	2.52	0.44
1:C:15:GLN:HG3	1:C:18:LEU:HG	2.00	0.44
1:A:34:THR:HG21	2:B:28:THR:HG23	2.00	0.44
1:G:130:PRO:HG2	1:G:136:HIS:CE1	2.52	0.44
1:G:113:SER:OG	1:G:115:THR:HG23	2.18	0.44
1:G:71:ILE:HG12	2:H:35:HIS:CD2	2.52	0.43
1:C:65:THR:HA	2:D:41:TYR:O	2.18	0.43
1:E:80:ALA:HB3	2:F:31:GLU:HB2	2.00	0.43
1:E:125:ASN:ND2	3:E:182:GYP:O4	2.51	0.43
1:E:21:GLN:HE21	1:E:43:ARG:NE	2.14	0.43
2:F:4:TYR:CD1	2:F:4:TYR:N	2.82	0.43
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.54	0.43
1:E:12:GLY:HA3	6:G:959:HOH:O	2.18	0.43
1:G:140:ASP:HB3	1:G:143:SER:O	2.18	0.43
1:C:79:VAL:HG22	1:C:122:THR:HB	2.01	0.43
1:C:28:LYS:HA	1:C:28:LYS:HD2	1.71	0.43
2:F:4:TYR:HH	5:F:689:MN:MN	1.40	0.43
1:A:144:ILE:HG13	1:A:144:ILE:O	2.19	0.43
2:D:10:VAL:HG13	2:D:10:VAL:O	2.18	0.43
1:G:132:ASN:ND2	1:G:134:ASP:HB2	2.34	0.42
1:E:53:TRP:HA	1:E:60:VAL:HA	2.01	0.42
1:A:175:VAL:O	2:B:5:THR:HA	2.19	0.42
1:G:80:ALA:CB	2:H:31:GLU:HB2	2.49	0.42
2:H:10:VAL:HA	2:H:11:PRO:HD2	1.79	0.42
1:C:155:GLN:HB2	1:C:179:TYR:CE1	2.55	0.42
1:E:128:TRP:HB2	1:E:145:LYS:CG	2.50	0.42
1:G:97:GLY:HA2	2:H:27:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:ND2	6:A:292:HOH:O	2.52	0.42
1:G:179:TYR:O	2:H:2:THR:N	2.53	0.42
1:E:84:THR:HG22	1:E:85:PHE:O	2.19	0.42
2:F:33:ALA:O	2:F:35:HIS:CD2	2.72	0.42
1:E:117:ALA:HB3	1:E:140:ASP:HB2	2.01	0.42
1:E:38:ARG:HD3	2:F:32:PHE:HE1	1.82	0.41
1:G:167:ASN:ND2	1:G:170:THR:H	2.18	0.41
3:C:182:GYP:C5	3:C:182:GYP:H7C3	2.51	0.41
1:C:167:ASN:ND2	1:C:170:THR:HG23	2.35	0.41
1:E:52:ILE:HD13	2:F:20:VAL:HG21	2.01	0.41
1:G:75:ASN:ND2	1:G:75:ASN:N	2.68	0.41
1:G:88:ALA:HB2	1:G:115:THR:HB	2.03	0.41
1:G:35:LYS:HD3	1:G:35:LYS:HA	1.90	0.41
1:C:33:LEU:HD12	1:C:33:LEU:HA	1.86	0.41
1:C:89:PRO:HD2	1:C:115:THR:HG22	2.02	0.41
1:A:68:THR:HA	1:A:160:ALA:O	2.20	0.41
1:A:49:PRO:HG2	1:C:16:GLN:O	2.20	0.41
2:D:17:PRO:HD2	2:D:20:VAL:HG12	2.02	0.41
1:A:19:ILE:O	1:A:44:ALA:HA	2.21	0.41
1:E:35:LYS:HE2	1:E:35:LYS:HA	2.02	0.40
1:C:178:THR:HB	2:D:3:SER:OG	2.21	0.40
1:C:123:PHE:CD2	3:C:182:GYP:H6C1	2.56	0.40
1:G:12:GLY:O	1:G:26:THR:HG21	2.22	0.40
2:F:17:PRO:HG2	2:F:20:VAL:HG12	2.02	0.40
1:E:66:SER:HB3	1:E:163:VAL:HG22	2.02	0.40
2:B:10:VAL:HG12	2:B:12:LEU:HD12	2.04	0.40
1:G:47:SER:O	2:H:21:ARG:NH1	2.54	0.40
1:A:34:THR:HG22	1:A:35:LYS:O	2.22	0.40
2:B:33:ALA:O	2:B:35:HIS:CD2	2.75	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	178/181 (98%)	172 (97%)	5 (3%)	1 (1%)	30 29
1	C	178/181 (98%)	164 (92%)	13 (7%)	1 (1%)	30 29
1	E	178/181 (98%)	165 (93%)	11 (6%)	2 (1%)	17 14
1	G	178/181 (98%)	164 (92%)	10 (6%)	4 (2%)	8 4
2	B	45/52 (86%)	43 (96%)	2 (4%)	0	100 100
2	D	45/52 (86%)	44 (98%)	1 (2%)	0	100 100
2	F	45/52 (86%)	41 (91%)	4 (9%)	0	100 100
2	H	45/52 (86%)	43 (96%)	2 (4%)	0	100 100
All	All	892/932 (96%)	836 (94%)	48 (5%)	8 (1%)	21 19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	28	LYS
1	C	28	LYS
1	G	39	ASN
1	E	28	LYS
1	E	111	LYS
1	A	99	GLY
1	G	130	PRO
1	G	8	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	154/155 (99%)	135 (88%)	19 (12%)	6 5
1	C	154/155 (99%)	137 (89%)	17 (11%)	8 7
1	E	154/155 (99%)	130 (84%)	24 (16%)	3 2
1	G	154/155 (99%)	128 (83%)	26 (17%)	2 2
2	B	40/44 (91%)	40 (100%)	0	100 100
2	D	39/44 (89%)	37 (95%)	2 (5%)	29 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	40/44 (91%)	37 (92%)	3 (8%)	17 17
2	H	39/44 (89%)	38 (97%)	1 (3%)	54 66
All	All	774/796 (97%)	682 (88%)	92 (12%)	6 5

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	30	ARG
1	A	35	LYS
1	A	37	VAL
1	A	47	SER
1	A	50	ILE
1	A	57	THR
1	A	60	VAL
1	A	66	SER
1	A	68	THR
1	A	81	ASP
1	A	84	THR
1	A	111	LYS
1	A	126	THR
1	A	130	PRO
1	A	131	SER
1	A	148	ASN
1	A	152	TRP
1	A	154	LEU
1	C	33	LEU
1	C	41	VAL
1	C	43	ARG
1	C	52	ILE
1	C	56	LYS
1	C	72	ASP
1	C	79	VAL
1	C	81	ASP
1	C	101	LEU
1	C	116	VAL
1	C	131	SER
1	C	141	VAL
1	C	145	LYS
1	C	149	THR
1	C	162	VAL

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Mol	Chain	Res	Type
1	C	176	SER
1	C	178	THR
2	D	8	GLU
2	D	36	GLU
1	E	3	THR
1	E	9	THR
1	E	14	ASP
1	E	28	LYS
1	E	29	GLU
1	E	32	THR
1	E	34	THR
1	E	37	VAL
1	E	38	ARG
1	E	50	ILE
1	E	52	ILE
1	E	57	THR
1	E	60	VAL
1	E	68	THR
1	E	72	ASP
1	E	76	SER
1	E	81	ASP
1	E	96	THR
1	E	103	VAL
1	E	111	LYS
1	E	131	SER
1	E	146	SER
1	E	148	ASN
1	E	154	LEU
2	F	14	GLU
2	F	16	VAL
2	F	41	TYR
1	G	7	SER
1	G	10	LYS
1	G	28	LYS
1	G	29	GLU
1	G	40	THR
1	G	41	VAL
1	G	51	HIS
1	G	54	ASP
1	G	66	SER
1	G	72	ASP
1	G	75	ASN

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Mol	Chain	Res	Type
1	G	76	SER
1	G	77	TYR
1	G	79	VAL
1	G	81	ASP
1	G	93	LYS
1	G	101	LEU
1	G	106	SER
1	G	114	GLN
1	G	115	THR
1	G	116	VAL
1	G	141	VAL
1	G	143	SER
1	G	149	THR
1	G	159	GLU
1	G	177	LEU
2	H	10	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	39	ASN
1	A	59	ASN
2	B	7	ASN
2	B	35	HIS
2	B	43	HIS
1	C	142	ASN
1	E	16	GLN
1	E	21	GLN
1	E	125	ASN
1	E	148	ASN
2	F	35	HIS
2	F	43	HIS
1	G	51	HIS
1	G	75	ASN
1	G	78	ASN
1	G	161	ASN
1	G	167	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	GYP	A	182	-	13,13,13	0.90	0	18,18,18	1.66	4 (22%)
3	GYP	C	182	-	13,13,13	0.79	0	18,18,18	1.63	3 (16%)
3	GYP	E	182	-	13,13,13	0.95	1 (7%)	18,18,18	1.61	4 (22%)
3	GYP	G	182	-	13,13,13	0.70	0	18,18,18	1.16	1 (5%)

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
3	GYP	A	182	-	-	0/4/24/24	0/1/1/1
3	GYP	C	182	-	-	0/4/24/24	0/1/1/1
3	GYP	E	182	-	-	0/4/24/24	0/1/1/1
3	GYP	G	182	-	-	0/4/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	182	GYP	O1-C1	2.04	1.43	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	182	GYP	C6-C5-C4	-4.20	102.67	113.02
3	C	182	GYP	C4-C3-C2	-4.03	103.28	110.79
3	A	182	GYP	C7-O1-C1	-3.99	106.77	113.29
3	C	182	GYP	O1-C1-C2	-3.50	104.08	108.21
3	E	182	GYP	C4-C3-C2	-3.13	104.94	110.79
3	A	182	GYP	O2-C2-C1	-2.30	104.98	110.02
3	A	182	GYP	O2-C2-C3	-2.09	105.63	110.34
3	E	182	GYP	O5-C5-C4	2.18	113.78	109.68
3	E	182	GYP	O3-C3-C2	2.32	115.55	110.34
3	C	182	GYP	O3-C3-C4	2.41	115.77	110.34
3	G	182	GYP	C1-O5-C5	2.45	118.49	113.75
3	A	182	GYP	C1-O5-C5	2.94	119.45	113.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	182	GYP	3	0
3	E	182	GYP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	180/181 (99%)	-1.04	0	100	100	11, 22, 35, 48	0
1	C	180/181 (99%)	-0.84	0	100	100	12, 30, 46, 57	0
1	E	180/181 (99%)	-0.86	0	100	100	13, 27, 44, 57	0
1	G	180/181 (99%)	-0.96	0	100	100	16, 26, 41, 51	0
2	B	47/52 (90%)	-1.11	0	100	100	6, 21, 31, 46	0
2	D	47/52 (90%)	-1.01	0	100	100	12, 28, 38, 41	0
2	F	47/52 (90%)	-0.98	0	100	100	9, 29, 41, 49	0
2	H	47/52 (90%)	-1.05	0	100	100	15, 23, 33, 39	0
All	All	908/932 (97%)	-0.95	0	100	100	6, 26, 42, 57	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MN	F	689	1/1	0.85	0.32	12.19	29,29,29,29	0
4	CA	C	458	1/1	0.96	0.16	2.55	36,36,36,36	0
4	CA	A	228	1/1	0.82	0.10	1.78	27,27,27,27	0
3	GYP	A	182	13/13	0.97	0.08	0.92	18,22,25,28	0
3	GYP	E	182	13/13	0.93	0.10	0.90	32,38,45,46	0
3	GYP	C	182	13/13	0.92	0.10	0.41	40,43,46,49	0
3	GYP	G	182	13/13	0.96	0.08	0.06	27,30,32,34	0
4	CA	E	688	1/1	0.96	0.08	-0.33	56,56,56,56	0
4	CA	G	918	1/1	0.97	0.06	-1.28	33,33,33,33	0
5	MN	C	459	1/1	0.97	0.04	-2.52	41,41,41,41	0
5	MN	G	919	1/1	0.98	0.04	-2.58	28,28,28,28	0
5	MN	A	229	1/1	0.99	0.03	-2.62	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.