Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:23 PM BST

PDB ID	:	4N2X
Title	:	Crystal Structure of DL-2-haloacid dehalogenase
Authors	:	Siwek, A.; Omi, R.; Hirotsu, K.; Jitsumori, K.; Esaki, N.; Kurihara, T.; Paneth, P.
Deposited on	:	2013-10-06
Resolution	:	1.70 Å(reported)

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

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

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

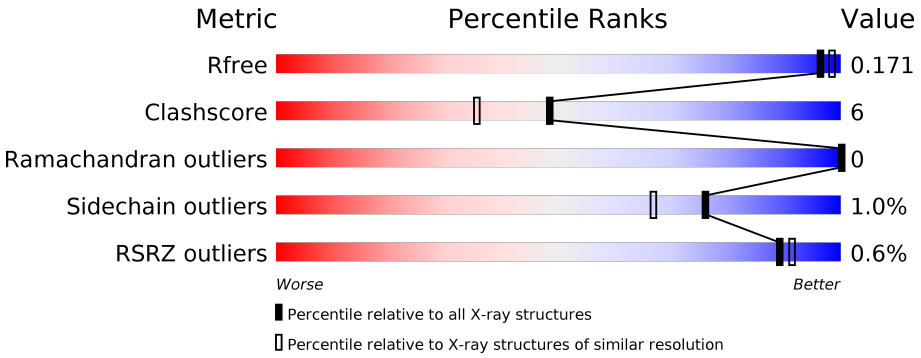
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	301	82% 15%
1	B	301	83% 14%
1	D	301	81% 17%
1	E	301	80% 18%
1	F	301	81% 16%
1	G	301	80% 16%

2 Entry composition

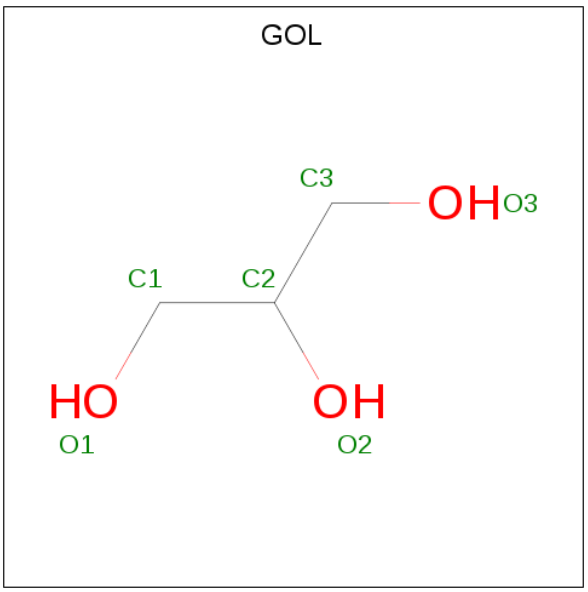
There are 3 unique types of molecules in this entry. The entry contains 17336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DL-2-haloacid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	4	0
			2399	1532	424	438	5			
1	B	298	Total	C	N	O	S	0	4	0
			2388	1525	422	436	5			
1	D	298	Total	C	N	O	S	0	2	0
			2388	1524	421	438	5			
1	E	298	Total	C	N	O	S	0	2	0
			2391	1525	424	437	5			
1	F	298	Total	C	N	O	S	0	4	0
			2405	1534	427	439	5			
1	G	298	Total	C	N	O	S	0	6	0
			2411	1538	427	441	5			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

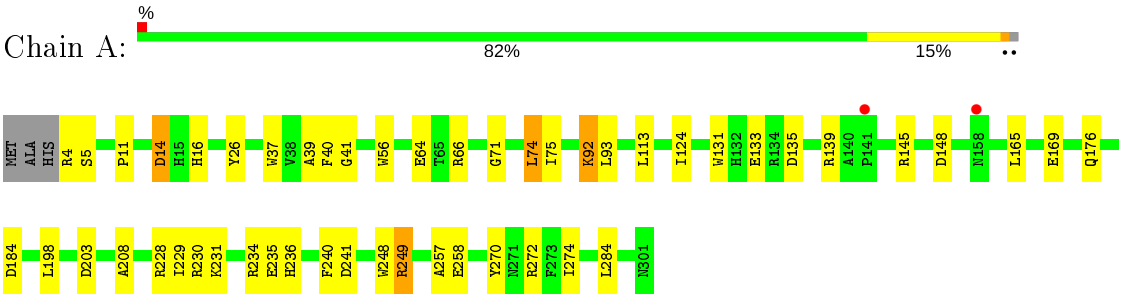
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	488	Total O 488 488	0	0
3	B	469	Total O 469 469	0	0
3	D	486	Total O 486 486	0	0
3	E	499	Total O 499 499	0	0
3	F	468	Total O 468 468	0	0
3	G	472	Total O 472 472	0	0

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.

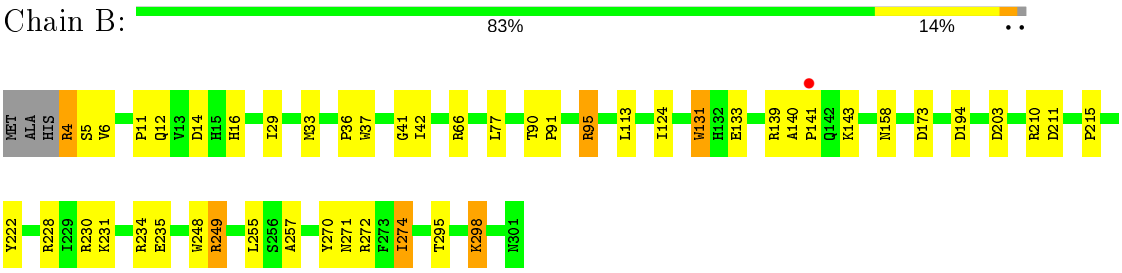
- Molecule 1: DL-2-haloacid dehalogenase

Chain A:



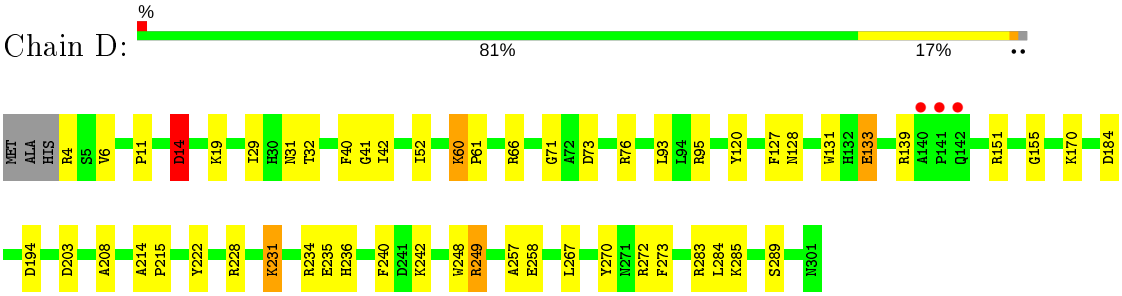
- Molecule 1: DL-2-haloacid dehalogenase

Chain B:



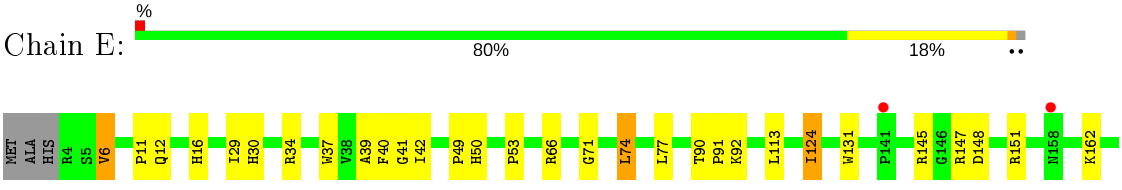
- Molecule 1: DL-2-haloacid dehalogenase

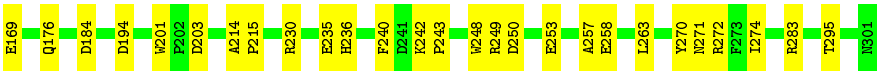
Chain D:



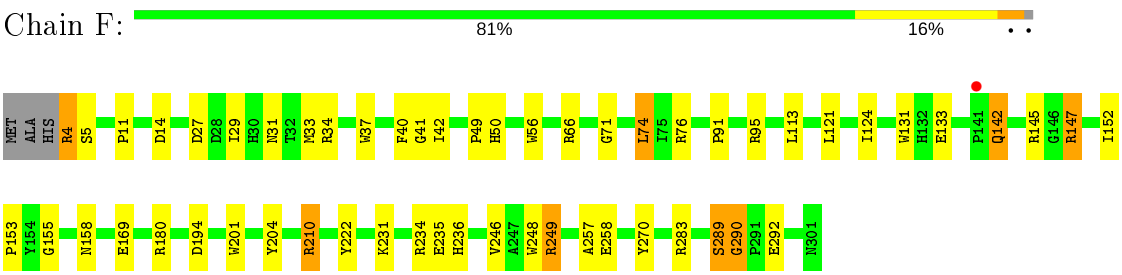
- Molecule 1: DL-2-haloacid dehalogenase

Chain E:

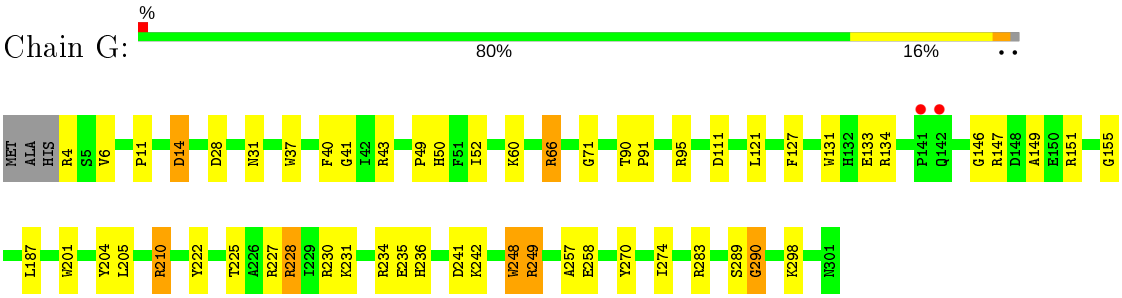




• Molecule 1: DL-2-haloacid dehalogenase



• Molecule 1: DL-2-haloacid dehalogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	182.57Å 182.57Å 112.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.70 42.27 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.70) 99.9 (42.27-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.20 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.135 , 0.172 0.134 , 0.171	Depositor DCC
R_{free} test set	23015 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å^2)	10.4	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.074 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17336	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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 57.02 % 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 2.5153e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	1.19	4/2470 (0.2%)	1.45	29/3353 (0.9%)
1	B	1.17	3/2459 (0.1%)	1.38	23/3340 (0.7%)
1	D	1.20	6/2453 (0.2%)	1.46	27/3332 (0.8%)
1	E	1.18	3/2456 (0.1%)	1.38	18/3335 (0.5%)
1	F	1.22	7/2476 (0.3%)	1.47	27/3361 (0.8%)
1	G	1.20	7/2488 (0.3%)	1.48	29/3377 (0.9%)
All	All	1.19	30/14802 (0.2%)	1.44	153/20098 (0.8%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	258	GLU	CD-OE2	-8.66	1.16	1.25
1	A	258	GLU	CD-OE2	-8.56	1.16	1.25
1	G	201	TRP	CD2-CE2	8.34	1.51	1.41
1	F	66	ARG	CZ-NH1	8.18	1.43	1.33
1	A	64	GLU	CD-OE1	-7.95	1.17	1.25
1	F	249	ARG	CD-NE	-7.82	1.33	1.46
1	D	6	VAL	N-CA	-7.24	1.31	1.46
1	F	201	TRP	CD2-CE2	7.16	1.50	1.41
1	G	248	TRP	CD2-CE2	7.15	1.50	1.41
1	G	66	ARG	CZ-NH2	7.03	1.42	1.33
1	G	249	ARG	CD-NE	-6.91	1.34	1.46
1	A	249	ARG	CD-NE	-6.83	1.34	1.46
1	B	249	ARG	CD-NE	-6.38	1.35	1.46
1	F	258	GLU	CD-OE2	-6.30	1.18	1.25
1	B	66	ARG	CZ-NH1	6.29	1.41	1.33
1	E	6	VAL	N-CA	-6.14	1.34	1.46
1	D	258	GLU	CD-OE2	-5.87	1.19	1.25
1	D	249	ARG	CZ-NH2	-5.84	1.25	1.33
1	G	227	ARG	CZ-NH1	5.62	1.40	1.33
1	G	258	GLU	CD-OE2	-5.43	1.19	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	37	TRP	CD2-CE2	5.33	1.47	1.41
1	B	131	TRP	CD2-CE2	5.31	1.47	1.41
1	D	249	ARG	CD-NE	-5.28	1.37	1.46
1	F	210[A]	ARG	CZ-NH1	-5.26	1.26	1.33
1	F	210[B]	ARG	CZ-NH1	-5.26	1.26	1.33
1	E	201	TRP	NE1-CE2	-5.21	1.30	1.37
1	D	133	GLU	CD-OE1	-5.16	1.20	1.25
1	F	56	TRP	CG-CD1	5.16	1.44	1.36
1	D	151	ARG	CZ-NH2	5.13	1.39	1.33
1	A	56	TRP	CD2-CE2	5.03	1.47	1.41

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	249	ARG	NE-CZ-NH1	21.21	130.91	120.30
1	G	249	ARG	NE-CZ-NH2	-20.36	110.12	120.30
1	D	249	ARG	NE-CZ-NH2	-18.58	111.01	120.30
1	D	249	ARG	NE-CZ-NH1	17.33	128.97	120.30
1	A	249	ARG	NE-CZ-NH2	-17.32	111.64	120.30
1	F	210[A]	ARG	NE-CZ-NH2	15.11	127.86	120.30
1	F	210[B]	ARG	NE-CZ-NH2	15.11	127.86	120.30
1	F	249	ARG	NE-CZ-NH2	-14.67	112.96	120.30
1	F	249	ARG	NE-CZ-NH1	14.24	127.42	120.30
1	B	249	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	A	249	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	E	148	ASP	CB-CG-OD2	-10.93	108.47	118.30
1	G	151	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	F	210[A]	ARG	NE-CZ-NH1	-10.58	115.01	120.30
1	F	210[B]	ARG	NE-CZ-NH1	-10.58	115.01	120.30
1	G	234	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	A	228	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	40	PHE	CB-CG-CD2	-9.90	113.87	120.80
1	B	249	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	F	66	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	B	66	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	B	14	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	B	4	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	F	234	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	F	4	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	G	283	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	G	234	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	A	148	ASP	CB-CG-OD2	-8.12	110.99	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	228	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	234	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	D	40	PHE	CB-CG-CD2	-7.83	115.31	120.80
1	F	289[A]	SER	CB-CA-C	7.62	124.57	110.10
1	F	289[B]	SER	CB-CA-C	7.62	124.57	110.10
1	F	283	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	E	272	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	198	LEU	CB-CG-CD1	-7.46	98.32	111.00
1	E	272	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	120	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	E	74	LEU	CB-CG-CD2	-7.29	98.61	111.00
1	B	274	ILE	CG1-CB-CG2	-7.23	95.49	111.40
1	E	6	VAL	CG1-CB-CG2	7.19	122.41	110.90
1	B	95	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	D	283	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	D	127	PHE	CB-CG-CD2	-7.12	115.82	120.80
1	E	230	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	G	40	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	G	14	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	D	228	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	272	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	E	263	LEU	CB-CG-CD1	-6.79	99.45	111.00
1	D	139	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	D	170	LYS	CD-CE-NZ	-6.77	96.12	111.70
1	G	241	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	135	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	B	222	TYR	CB-CG-CD1	-6.74	116.96	121.00
1	B	14	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	272	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	230	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	145	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	G	230	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	F	180	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	F	74	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	D	242	LYS	CD-CE-NZ	6.49	126.63	111.70
1	B	298	LYS	CD-CE-NZ	-6.47	96.83	111.70
1	D	283	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	234	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	D	184	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	D	66	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	241	ASP	CB-CG-OD1	6.36	124.03	118.30
1	D	203	ASP	CB-CG-OD2	6.36	124.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	273	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	B	230	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	173	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	G	222	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	A	92[A]	LYS	CD-CE-NZ	6.28	126.14	111.70
1	A	92[B]	LYS	CD-CE-NZ	6.28	126.14	111.70
1	B	228	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	14	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	203	ASP	CB-CG-OD1	6.13	123.81	118.30
1	F	290	GLY	N-CA-C	-6.13	97.78	113.10
1	G	28	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	F	40	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	G	204	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	B	33	MET	CA-CB-CG	-6.00	103.09	113.30
1	A	26	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	B	228	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	139	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	D	73	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	234	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	E	283	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	240	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	D	76	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	222	TYR	CB-CG-CD1	-5.76	117.55	121.00
1	A	4	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	D	231	LYS	CD-CE-NZ	-5.73	98.53	111.70
1	E	74	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	E	40	PHE	CB-CG-CD2	-5.68	116.83	120.80
1	E	151	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	230	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	E	240	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	G	127	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	G	290	GLY	N-CA-C	-5.64	99.00	113.10
1	A	74	LEU	CB-CG-CD1	-5.62	101.44	111.00
1	G	249	ARG	CD-NE-CZ	5.62	131.47	123.60
1	F	194	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	203	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	40	PHE	CB-CG-CD1	5.61	124.73	120.80
1	B	234	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	76	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	E	184	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	F	234	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	139	ARG	CG-CD-NE	-5.53	100.18	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	33	MET	CA-CB-CG	-5.53	103.90	113.30
1	G	6	VAL	N-CA-CB	-5.52	99.35	111.50
1	B	211	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	184	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	66	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	203	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	40	PHE	CB-CG-CD1	5.42	124.59	120.80
1	F	34	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	255	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	E	34	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	240	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	G	40	PHE	CB-CG-CD1	5.40	124.58	120.80
1	A	165	LEU	CB-CG-CD1	5.38	120.15	111.00
1	F	145	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	F	40	PHE	CB-CG-CD1	5.37	124.56	120.80
1	G	121	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	F	27	ASP	CB-CG-OD1	5.36	123.12	118.30
1	E	203	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	G	210[A]	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	G	210[B]	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	G	14	ASP	CB-CG-OD1	5.32	123.09	118.30
1	G	111	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	234	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	203	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	E	249	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	14	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	F	222	TYR	CZ-CE2-CD2	-5.21	115.11	119.80
1	B	203	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	G	43	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	60	LYS	CD-CE-NZ	-5.17	99.80	111.70
1	F	204	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	E	124	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	A	93	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	D	6	VAL	CG1-CB-CG2	5.12	119.09	110.90
1	G	187	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	G	134	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	272	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	F	147	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	G	60	LYS	CD-CE-NZ	-5.06	100.05	111.70
1	G	66	ARG	CD-NE-CZ	5.05	130.67	123.60
1	A	40	PHE	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2399	0	2398	28	0
1	B	2388	0	2380	27	0
1	D	2388	0	2375	25	0
1	E	2391	0	2385	34	0
1	F	2405	0	2404	33	0
1	G	2411	0	2414	34	0
2	A	12	0	16	0	0
2	B	12	0	16	1	0
2	D	12	0	16	0	0
2	E	12	0	16	0	0
2	F	12	0	16	0	0
2	G	12	0	16	0	0
3	A	488	0	0	9	0
3	B	469	0	0	7	0
3	D	486	0	0	4	1
3	E	499	0	0	6	0
3	F	468	0	0	13	0
3	G	472	0	0	19	1
All	All	17336	0	14452	172	1

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 6.

All (172) 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:E:124:ILE:HG13	1:E:274:ILE:CD1	1.53	1.36
1:D:289:SER:HB3	3:D:693:HOH:O	1.06	1.23
1:F:210[A]:ARG:HD2	3:F:683:HOH:O	1.35	1.23
1:E:235:GLU:HG3	3:G:677:HOH:O	1.38	1.19
1:G:274:ILE:HG23	3:G:728:HOH:O	1.51	1.10
1:E:124:ILE:HG13	1:E:274:ILE:HD12	1.26	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:ILE:HG23	3:E:705:HOH:O	1.55	1.05
1:E:124:ILE:HG13	1:E:274:ILE:HD13	1.42	0.98
1:B:133:GLU:OE1	1:B:249:ARG:HD3	1.61	0.98
1:A:92[B]:LYS:HG3	3:A:572:HOH:O	1.67	0.93
1:G:133:GLU:OE1	1:G:249:ARG:HD3	1.68	0.92
1:F:290:GLY:N	3:F:719:HOH:O	2.00	0.92
1:D:133:GLU:OE2	1:D:249:ARG:HD3	1.70	0.92
1:F:133:GLU:OE2	1:F:249:ARG:HD3	1.71	0.90
1:G:289[A]:SER:CB	3:G:755:HOH:O	2.17	0.90
1:G:289[A]:SER:HB2	3:G:755:HOH:O	1.71	0.90
1:G:290:GLY:N	3:G:755:HOH:O	2.00	0.90
1:F:289[B]:SER:CB	3:F:719:HOH:O	2.19	0.90
1:F:289[B]:SER:HB2	3:F:719:HOH:O	1.72	0.89
1:A:133:GLU:OE1	1:A:249:ARG:HD3	1.73	0.89
1:G:289[A]:SER:CA	3:G:755:HOH:O	2.16	0.87
1:G:289[B]:SER:CA	3:G:755:HOH:O	2.18	0.85
1:E:124:ILE:CG1	1:E:274:ILE:CD1	2.49	0.85
1:F:289[A]:SER:CA	3:F:719:HOH:O	2.25	0.84
1:A:124:ILE:HG21	1:A:274:ILE:HG21	1.61	0.82
1:F:289[B]:SER:CA	3:F:719:HOH:O	2.23	0.82
1:F:210[B]:ARG:NH1	3:F:683:HOH:O	1.78	0.81
1:B:143:LYS:HE2	3:B:595:HOH:O	1.80	0.80
1:A:92[A]:LYS:HD3	3:A:714:HOH:O	1.84	0.77
1:B:124:ILE:HG21	1:B:274:ILE:CG2	2.15	0.77
1:G:66:ARG:NE	3:G:911:HOH:O	1.88	0.74
1:A:124:ILE:HG21	1:A:274:ILE:CG2	2.17	0.74
1:B:124:ILE:HG21	1:B:274:ILE:HG21	1.71	0.72
1:B:298:LYS:CE	3:B:767:HOH:O	2.35	0.71
1:G:289[B]:SER:CB	3:G:755:HOH:O	2.37	0.70
1:D:14:ASP:OD2	3:D:817:HOH:O	2.11	0.69
1:F:289[A]:SER:CB	3:F:719:HOH:O	2.43	0.67
1:E:124:ILE:CG1	1:E:274:ILE:HD12	2.14	0.67
1:G:289[B]:SER:HB3	3:G:755:HOH:O	1.95	0.65
1:A:92[A]:LYS:CE	3:A:714:HOH:O	2.45	0.63
1:A:131:TRP:CE2	1:A:248:TRP:HB3	2.34	0.62
1:A:124:ILE:CG2	1:A:274:ILE:HG21	2.30	0.62
1:F:131:TRP:CE2	1:F:248:TRP:HB3	2.35	0.62
1:D:11:PRO:HB3	1:E:257:ALA:HB1	1.80	0.62
1:A:257:ALA:HB1	1:B:11:PRO:HB3	1.83	0.61
1:B:124:ILE:CG2	1:B:274:ILE:HG21	2.30	0.61
1:D:131:TRP:CE2	1:D:248:TRP:HB3	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:CG1	1:E:274:ILE:HD13	2.25	0.60
1:D:257:ALA:HB1	1:E:11:PRO:HB3	1.83	0.59
1:B:210[B]:ARG:NE	3:B:937:HOH:O	2.13	0.59
1:A:11:PRO:HB3	1:B:257:ALA:HB1	1.84	0.59
1:A:92[B]:LYS:CG	3:A:572:HOH:O	2.38	0.59
1:F:292[A]:GLU:HG2	3:F:922:HOH:O	2.03	0.58
1:F:257:ALA:HB1	1:G:11:PRO:HB3	1.86	0.57
1:F:289[A]:SER:HB3	3:F:719:HOH:O	2.04	0.57
1:B:298:LYS:NZ	3:B:767:HOH:O	2.01	0.56
1:G:131:TRP:CE2	1:G:248:TRP:HB3	2.41	0.56
1:B:91:PRO:O	1:B:95:ARG:HG3	2.05	0.55
1:F:292[A]:GLU:CG	3:F:922:HOH:O	2.54	0.55
1:F:31:ASN:HD22	1:F:155:GLY:HA2	1.73	0.54
3:B:530:HOH:O	1:E:92:LYS:HE2	2.07	0.54
1:F:91:PRO:O	1:F:95:ARG:HG3	2.08	0.53
1:B:124:ILE:HG21	1:B:274:ILE:HG22	1.91	0.53
1:B:131:TRP:CE2	1:B:248:TRP:HB3	2.43	0.53
1:E:131:TRP:CE2	1:E:248:TRP:HB3	2.43	0.53
1:G:66:ARG:NH2	3:G:911:HOH:O	2.40	0.53
1:A:92[A]:LYS:CD	3:A:714:HOH:O	2.50	0.53
1:D:128:ASN:HD22	1:D:267:LEU:HB3	1.75	0.52
1:F:41:GLY:HA2	1:F:270:TYR:CZ	2.44	0.52
1:E:39:ALA:HB3	3:E:729:HOH:O	2.10	0.52
1:F:49:PRO:HB2	1:F:50:HIS:CD2	2.44	0.51
1:F:4:ARG:HG2	1:F:5:SER:N	2.25	0.51
1:A:41:GLY:HA2	1:A:270:TYR:CZ	2.45	0.51
1:G:31:ASN:HD22	1:G:155:GLY:HA2	1.76	0.51
1:G:210[A]:ARG:NH1	3:G:955:HOH:O	2.21	0.51
1:A:270:TYR:O	1:A:274:ILE:HG22	2.10	0.51
1:F:37:TRP:CH2	1:F:113:LEU:HA	2.46	0.51
1:G:66:ARG:CZ	3:G:911:HOH:O	2.46	0.51
1:F:142:GLN:NE2	1:F:142:GLN:H	2.09	0.50
1:F:29:ILE:HD13	1:F:42:ILE:HD13	1.93	0.50
1:E:242:LYS:HB2	1:E:243:PRO:CD	2.41	0.50
1:G:149:ALA:HB3	3:G:622:HOH:O	2.13	0.49
1:D:71:GLY:HA3	1:D:236:HIS:CD2	2.48	0.49
1:G:149:ALA:CB	3:G:622:HOH:O	2.60	0.48
1:A:39:ALA:HB3	3:A:715:HOH:O	2.13	0.48
1:A:37:TRP:CH2	1:A:113:LEU:HA	2.49	0.48
1:G:146:GLY:O	3:G:622:HOH:O	2.20	0.48
1:F:71:GLY:HA3	1:F:236:HIS:CD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HA	1:B:295:THR:HB	1.94	0.48
1:F:169:GLU:HG3	3:F:690:HOH:O	2.14	0.48
1:G:31:ASN:ND2	1:G:155:GLY:HA2	2.29	0.47
1:G:41:GLY:HA2	1:G:270:TYR:CZ	2.49	0.47
1:E:169:GLU:HG3	3:E:728:HOH:O	2.15	0.47
1:B:95:ARG:HA	1:G:147:ARG:NH1	2.30	0.47
1:A:5:SER:HB2	1:A:176:GLN:OE1	2.15	0.47
1:A:92[B]:LYS:NZ	3:A:728:HOH:O	2.46	0.47
1:B:41:GLY:HA2	1:B:270:TYR:CZ	2.50	0.47
1:A:16:HIS:H	1:A:16:HIS:CD2	2.32	0.46
1:E:30:HIS:CD2	1:E:162:LYS:HE2	2.50	0.46
1:G:49:PRO:HB2	1:G:50:HIS:CD2	2.50	0.46
1:G:71:GLY:HA3	1:G:236:HIS:CD2	2.51	0.46
1:B:90:THR:HB	1:B:91:PRO:HD3	1.98	0.46
1:G:52:ILE:HA	1:G:52:ILE:HD13	1.86	0.46
1:E:66:ARG:O	1:E:66:ARG:HD3	2.16	0.46
1:E:90:THR:HB	1:E:91:PRO:HD3	1.98	0.46
1:A:208:ALA:HB1	1:A:284:LEU:HD22	1.98	0.45
1:G:205:LEU:HA	1:G:205:LEU:HD23	1.82	0.45
1:B:12:GLN:O	3:B:930:HOH:O	2.21	0.45
1:A:231:LYS:CE	1:A:235[A]:GLU:OE2	2.65	0.45
1:E:12:GLN:O	3:E:554:HOH:O	2.21	0.45
1:B:231:LYS:HE3	1:B:235[A]:GLU:OE2	2.17	0.45
1:E:16:HIS:CD2	1:E:16:HIS:H	2.34	0.45
1:F:31:ASN:ND2	1:F:155:GLY:HA2	2.31	0.45
1:E:6:VAL:HB	1:E:176:GLN:HB3	1.99	0.44
1:D:52:ILE:HA	1:D:52:ILE:HD13	1.90	0.44
1:D:32:THR:HG21	1:D:60:LYS:HG3	1.99	0.44
1:F:131:TRP:HA	1:F:246:VAL:O	2.17	0.44
1:G:231:LYS:O	1:G:235[B]:GLU:HG3	2.17	0.44
1:B:140:ALA:HB1	1:B:141:PRO:HD2	2.00	0.44
1:D:194:ASP:N	1:D:194:ASP:OD2	2.50	0.44
1:E:37:TRP:CH2	1:E:113:LEU:HA	2.53	0.44
1:B:36:PRO:HD2	3:B:662:HOH:O	2.18	0.44
1:E:29:ILE:HD13	1:E:42:ILE:HD13	1.99	0.44
1:D:231:LYS:HE2	3:D:856:HOH:O	2.17	0.43
1:A:71:GLY:HA3	1:A:236:HIS:CD2	2.53	0.43
1:A:92[B]:LYS:NZ	3:A:985:HOH:O	2.51	0.43
1:F:11:PRO:HB3	1:G:257:ALA:HB1	2.00	0.43
1:G:90:THR:HB	1:G:91:PRO:HD3	1.99	0.43
1:E:194:ASP:OD2	1:E:194:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:PRO:HB2	1:E:50:HIS:CD2	2.53	0.43
1:E:242:LYS:HE2	3:E:681:HOH:O	2.18	0.43
1:A:14:ASP:OD2	3:A:978:HOH:O	2.21	0.43
1:F:121:LEU:HA	1:F:124:ILE:HG22	2.00	0.43
1:E:145:ARG:NH2	3:E:967:HOH:O	2.45	0.43
1:A:131:TRP:CD2	1:A:248:TRP:HB3	2.53	0.42
1:E:77:LEU:HA	1:E:295:THR:HB	2.01	0.42
1:G:225:THR:HG23	1:G:228:ARG:NH2	2.34	0.42
1:D:208:ALA:HB1	1:D:284:LEU:HD22	2.01	0.42
1:D:41:GLY:HA2	1:D:270:TYR:CZ	2.54	0.42
1:B:215:PRO:HG3	2:B:402:GOL:H31	2.02	0.42
1:B:158:ASN:H	1:B:158:ASN:ND2	2.17	0.42
1:D:29:ILE:HD13	1:D:42:ILE:HD13	2.01	0.42
1:D:4:ARG:NH1	1:E:250:ASP:OD1	2.41	0.42
1:D:231:LYS:O	1:D:235[A]:GLU:HG3	2.20	0.42
1:B:16:HIS:CD2	1:B:16:HIS:H	2.38	0.42
1:B:29:ILE:HD13	1:B:42:ILE:HD13	2.02	0.42
1:D:19:LYS:HA	1:D:19:LYS:HD3	1.87	0.42
1:E:74:LEU:HD12	1:E:74:LEU:HA	1.82	0.42
1:F:231:LYS:O	1:F:235[A]:GLU:HG3	2.19	0.42
1:E:41:GLY:HA2	1:E:270:TYR:CZ	2.54	0.41
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.91	0.41
1:E:147:ARG:NH1	1:G:95:ARG:HA	2.35	0.41
1:D:95:ARG:HB3	1:F:147:ARG:HD2	2.02	0.41
1:D:214:ALA:N	1:D:215:PRO:CD	2.84	0.41
1:E:214:ALA:N	1:E:215:PRO:CD	2.84	0.41
1:B:4:ARG:HG2	1:B:5:SER:N	2.34	0.41
1:D:95:ARG:CB	1:F:147:ARG:HD2	2.50	0.41
1:A:231:LYS:HE2	1:A:235[A]:GLU:OE2	2.20	0.41
1:F:152:ILE:HB	1:F:153:PRO:CD	2.51	0.41
1:G:131:TRP:CD2	1:G:248:TRP:HB3	2.56	0.41
1:F:131:TRP:CD2	1:F:248:TRP:HB3	2.55	0.41
1:A:74:LEU:HA	1:A:74:LEU:HD23	1.91	0.41
1:D:131:TRP:CZ2	1:D:248:TRP:HB3	2.56	0.41
1:A:75:ILE:HG23	1:A:229:ILE:HB	2.02	0.40
1:G:298:LYS:HE2	3:G:909:HOH:O	2.20	0.40
1:D:285:LYS:HE2	3:D:693:HOH:O	2.22	0.40
1:D:31:ASN:HD22	1:D:155:GLY:HA2	1.87	0.40
1:E:71:GLY:HA3	1:E:236:HIS:CD2	2.57	0.40
1:B:37:TRP:CH2	1:B:113:LEU:HA	2.56	0.40
1:G:242:LYS:HE3	3:G:694:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:896:HOH:O	3:G:582:HOH:O[4_665]	1.98	0.22

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	300/301 (100%)	296 (99%)	4 (1%)	0	100	100
1	B	300/301 (100%)	294 (98%)	6 (2%)	0	100	100
1	D	298/301 (99%)	293 (98%)	5 (2%)	0	100	100
1	E	298/301 (99%)	294 (99%)	4 (1%)	0	100	100
1	F	300/301 (100%)	296 (99%)	4 (1%)	0	100	100
1	G	302/301 (100%)	297 (98%)	5 (2%)	0	100	100
All	All	1798/1806 (100%)	1770 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	252/251 (100%)	251 (100%)	1 (0%)	91	87
1	B	250/251 (100%)	247 (99%)	3 (1%)	71	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	250/251 (100%)	248 (99%)	2 (1%)	81 74
1	E	251/251 (100%)	248 (99%)	3 (1%)	71 59
1	F	253/251 (101%)	249 (98%)	4 (2%)	62 48
1	G	255/251 (102%)	253 (99%)	2 (1%)	81 74
All	All	1511/1506 (100%)	1496 (99%)	15 (1%)	76 67

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	GLU
1	B	6	VAL
1	B	194	ASP
1	B	271	ASN
1	D	14	ASP
1	D	61	PRO
1	E	53	PRO
1	E	253	GLU
1	E	271	ASN
1	F	14	ASP
1	F	74	LEU
1	F	142	GLN
1	F	158	ASN
1	G	4	ARG
1	G	14	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	47	GLN
1	A	271	ASN
1	B	16	HIS
1	B	31	ASN
1	B	158	ASN
1	D	16	HIS
1	D	31	ASN
1	D	117	ASN
1	D	128	ASN
1	D	158	ASN
1	D	271	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	16	HIS
1	E	117	ASN
1	E	176	GLN
1	F	16	HIS
1	F	31	ASN
1	F	62	ASN
1	F	142	GLN
1	F	271	ASN
1	G	16	HIS
1	G	31	ASN
1	G	271	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 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	GOL	D	402	-	5,5,5	0.44	0	5,5,5	0.89	0
2	GOL	F	402	-	5,5,5	0.79	0	5,5,5	0.86	0
2	GOL	F	401	-	5,5,5	0.80	0	5,5,5	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	B	402	-	5,5,5	1.02	0	5,5,5	1.37	0
2	GOL	D	401	-	5,5,5	0.85	0	5,5,5	0.63	0
2	GOL	G	401	-	5,5,5	0.72	0	5,5,5	1.06	0
2	GOL	B	401	-	5,5,5	1.05	0	5,5,5	0.77	0
2	GOL	E	401	-	5,5,5	0.91	0	5,5,5	1.00	0
2	GOL	E	402	-	5,5,5	0.68	0	5,5,5	0.87	0
2	GOL	A	401	-	5,5,5	0.79	0	5,5,5	0.55	0
2	GOL	G	402	-	5,5,5	0.79	0	5,5,5	1.19	0
2	GOL	A	402	-	5,5,5	0.61	0	5,5,5	0.52	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	GOL	D	402	-	-	0/4/4/4	-
2	GOL	F	402	-	-	0/4/4/4	-
2	GOL	F	401	-	-	0/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	G	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	E	401	-	-	0/4/4/4	-
2	GOL	E	402	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	G	402	-	-	2/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	402	GOL	O1-C1-C2-O2
2	G	402	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	298/301 (99%)	-0.69	2 (0%)	87	90	5, 9, 23, 40	0
1	B	298/301 (99%)	-0.69	1 (0%)	94	94	5, 9, 24, 42	0
1	D	298/301 (99%)	-0.71	3 (1%)	82	85	5, 8, 22, 49	0
1	E	298/301 (99%)	-0.69	2 (0%)	87	90	4, 8, 22, 46	0
1	F	298/301 (99%)	-0.70	1 (0%)	94	94	5, 9, 25, 52	0
1	G	298/301 (99%)	-0.66	2 (0%)	87	90	5, 9, 23, 48	0
All	All	1788/1806 (99%)	-0.69	11 (0%)	89	91	4, 9, 23, 52	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	141	PRO	6.1
1	G	141	PRO	5.2
1	E	141	PRO	5.1
1	B	141	PRO	4.2
1	D	141	PRO	3.9
1	A	141	PRO	3.9
1	D	140	ALA	2.4
1	E	158	ASN	2.4
1	G	142	GLN	2.4
1	D	142	GLN	2.3
1	A	158	ASN	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	F	401	6/6	0.88	0.18	18,23,25,29	0
2	GOL	G	401	6/6	0.90	0.19	19,22,24,28	0
2	GOL	D	401	6/6	0.91	0.14	14,19,22,27	0
2	GOL	B	401	6/6	0.92	0.17	16,23,24,24	0
2	GOL	E	401	6/6	0.92	0.16	14,19,22,24	0
2	GOL	A	401	6/6	0.92	0.13	16,21,21,27	0
2	GOL	F	402	6/6	0.95	0.12	13,18,19,22	0
2	GOL	B	402	6/6	0.96	0.10	12,17,19,21	0
2	GOL	G	402	6/6	0.96	0.10	13,18,20,21	0
2	GOL	D	402	6/6	0.97	0.07	12,15,15,19	0
2	GOL	E	402	6/6	0.98	0.05	13,15,15,17	0
2	GOL	A	402	6/6	0.98	0.06	13,15,16,17	0

6.5 Other polymers (i)

There are no such residues in this entry.