



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:50 AM UTC

PDB ID : 4N2X / pdb_00004n2x
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

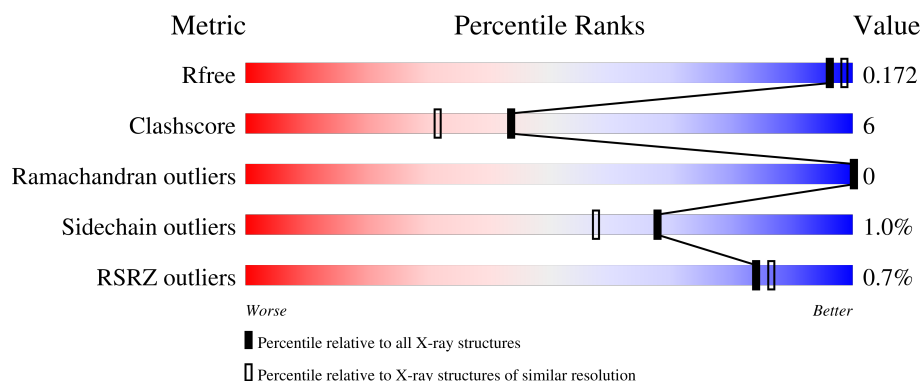
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	301	
1	D	301	
1	E	301	
1	F	301	

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Mol	Chain	Length	Quality of chain
1	G	301	% 81% 16% ..

2 Entry composition [i](#)

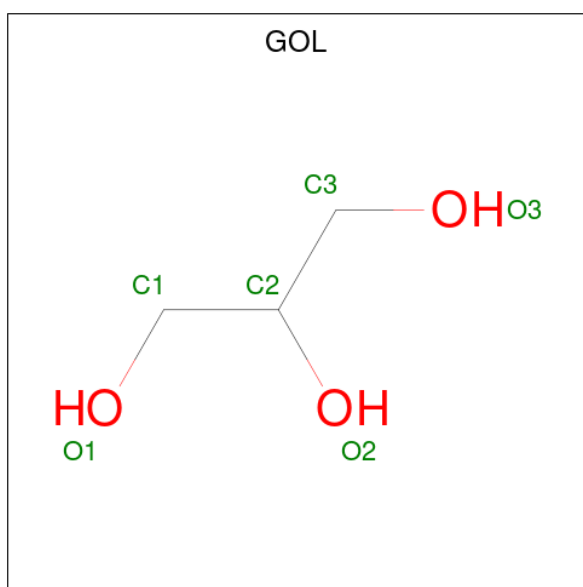
There are 3 unique types of molecules in this entry. The entry contains 17336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

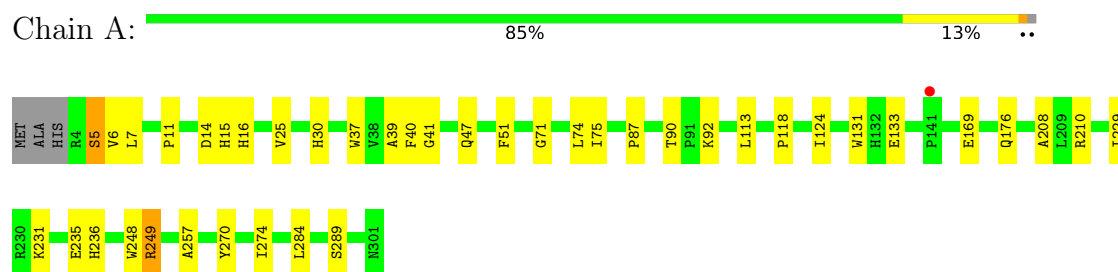
- Molecule 3 is water.

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

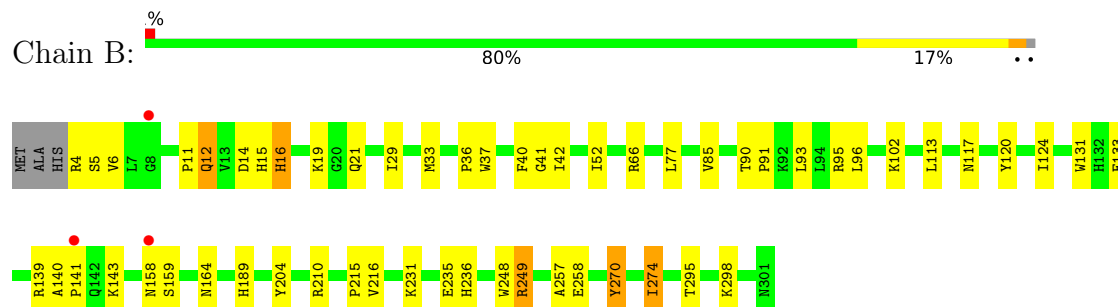
3 Residue-property plots

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.

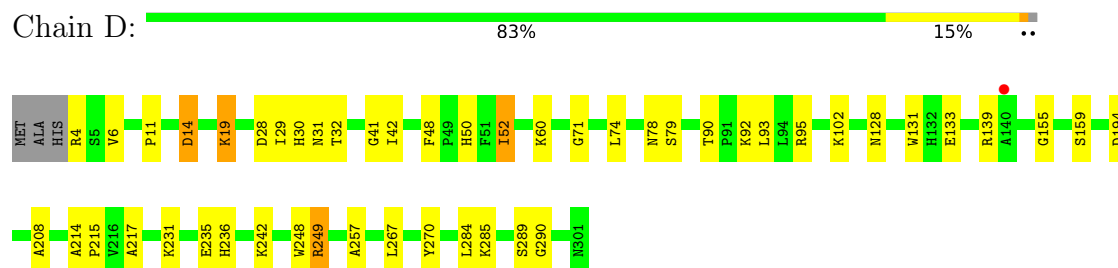
• Molecule 1: DL-2-haloacid dehalogenase



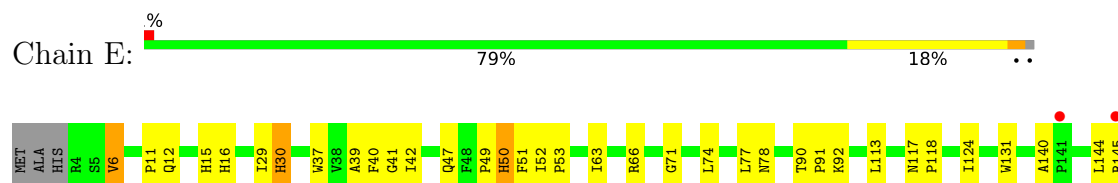
• Molecule 1: DL-2-haloacid dehalogenase



• Molecule 1: DL-2-haloacid dehalogenase



• Molecule 1: DL-2-haloacid dehalogenase





- Molecule 1: DL-2-haloacid dehalogenase

Chain F: 81% 16% ..



- Molecule 1: DL-2-haloacid dehalogenase

Chain G: 81% 16% ..



4 Data and refinement statistics

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 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.70) 99.8 (50.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.20 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.135 , 0.172 0.135 , 0.172	Depositor DCC
R_{free} test set	23015 reflections (9.91%)	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)	0.40 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.52	11/2470 (0.4%)	1.54	7/3353 (0.2%)
1	B	1.54	20/2459 (0.8%)	1.48	11/3340 (0.3%)
1	D	1.54	10/2453 (0.4%)	1.56	17/3332 (0.5%)
1	E	1.56	17/2456 (0.7%)	1.55	14/3335 (0.4%)
1	F	1.57	19/2476 (0.8%)	1.50	12/3361 (0.4%)
1	G	1.57	23/2488 (0.9%)	1.52	13/3377 (0.4%)
All	All	1.55	100/14802 (0.7%)	1.53	74/20098 (0.4%)

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	6	VAL	N-CA	-12.01	1.31	1.46
1	E	6	VAL	N-CA	-11.05	1.34	1.46
1	B	52	ILE	CA-CB	-10.69	1.48	1.54
1	F	249	ARG	CD-NE	-9.36	1.33	1.46
1	G	249	ARG	CD-NE	-8.24	1.34	1.46
1	A	249	ARG	CD-NE	-8.15	1.34	1.46
1	F	66	ARG	CZ-NH1	7.81	1.43	1.32
1	G	6	VAL	N-CA	-7.69	1.37	1.46
1	F	52	ILE	CA-CB	-7.61	1.50	1.54
1	E	63	ILE	C-O	-7.61	1.15	1.24
1	B	249	ARG	CD-NE	-7.60	1.35	1.46
1	E	52	ILE	C-O	-7.47	1.18	1.24
1	E	117	ASN	C-O	-7.16	1.17	1.24
1	E	242	LYS	N-CA	-7.11	1.39	1.46
1	A	7	LEU	C-O	-7.03	1.16	1.24
1	B	216	VAL	N-CA	-6.88	1.40	1.46
1	F	289[A]	SER	CA-C	6.86	1.55	1.52
1	F	289[B]	SER	CA-C	6.86	1.55	1.52
1	B	85	VAL	N-CA	-6.80	1.38	1.46
1	E	188	HIS	CE1-NE2	6.79	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	289[A]	SER	C-O	6.72	1.32	1.24
1	G	289[B]	SER	C-O	6.72	1.32	1.24
1	G	66	ARG	CZ-NH2	6.72	1.42	1.33
1	A	15	HIS	CG-CD2	6.67	1.43	1.35
1	D	50	HIS	ND1-CE1	6.64	1.39	1.32
1	G	117	ASN	C-O	-6.64	1.18	1.24
1	F	30	HIS	ND1-CE1	6.54	1.39	1.32
1	E	30	HIS	ND1-CE1	6.49	1.39	1.32
1	A	289	SER	CA-C	6.46	1.55	1.52
1	E	50	HIS	ND1-CE1	6.43	1.39	1.32
1	F	6	VAL	N-CA	-6.41	1.38	1.46
1	D	52	ILE	CA-CB	-6.36	1.50	1.54
1	B	15	HIS	CG-CD2	6.34	1.42	1.35
1	D	249	ARG	CD-NE	-6.27	1.37	1.46
1	G	224	GLU	N-CA	-6.26	1.38	1.46
1	D	249	ARG	CZ-NH2	-6.14	1.25	1.33
1	A	15	HIS	ND1-CE1	6.09	1.38	1.32
1	E	201	TRP	NE1-CE2	-6.07	1.30	1.37
1	B	66	ARG	CZ-NH1	6.06	1.41	1.32
1	A	51	PHE	N-CA	-6.00	1.39	1.46
1	G	289[A]	SER	C-N	-5.97	1.24	1.33
1	G	289[B]	SER	C-N	-5.97	1.24	1.33
1	G	50	HIS	CA-C	-5.93	1.44	1.52
1	B	120	TYR	C-O	-5.90	1.16	1.24
1	B	16	HIS	CE1-NE2	5.89	1.38	1.32
1	G	201	TRP	CD2-CE2	5.89	1.51	1.41
1	B	14	ASP	CG-OD1	5.88	1.36	1.25
1	F	15	HIS	CG-CD2	5.86	1.42	1.35
1	G	66	ARG	NE-CZ	5.80	1.39	1.33
1	F	15	HIS	ND1-CE1	5.78	1.38	1.32
1	E	300	THR	CA-C	-5.73	1.46	1.53
1	B	117	ASN	C-O	-5.68	1.19	1.24
1	A	30	HIS	ND1-CE1	5.67	1.38	1.32
1	B	236	HIS	CA-C	-5.60	1.45	1.52
1	F	117	ASN	C-O	-5.59	1.19	1.24
1	A	210	ARG	CD-NE	5.57	1.54	1.46
1	F	289[A]	SER	C-N	-5.56	1.25	1.33
1	F	289[B]	SER	C-N	-5.56	1.25	1.33
1	F	33	MET	N-CA	5.54	1.53	1.46
1	G	98	TRP	CA-C	-5.50	1.45	1.52
1	F	292[A]	GLU	C-O	-5.49	1.17	1.24
1	F	292[B]	GLU	C-O	-5.49	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	145	ARG	CA-C	-5.46	1.45	1.52
1	E	214	ALA	C-N	-5.46	1.28	1.34
1	B	12	GLN	CA-C	-5.44	1.46	1.52
1	G	227	ARG	CZ-NH1	5.44	1.40	1.32
1	G	11	PRO	CA-C	-5.43	1.46	1.52
1	E	289[A]	SER	C-N	-5.42	1.25	1.33
1	E	289[B]	SER	C-N	-5.42	1.25	1.33
1	G	189	HIS	CE1-NE2	5.41	1.38	1.32
1	A	118	PRO	C-O	-5.41	1.17	1.24
1	G	30	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	90	THR	N-CA	5.39	1.51	1.46
1	E	15	HIS	CB-CG	5.38	1.57	1.50
1	F	50	HIS	ND1-CE1	5.36	1.38	1.32
1	F	258	GLU	N-CA	-5.33	1.40	1.46
1	B	258	GLU	N-CA	-5.33	1.40	1.46
1	B	270	TYR	C-O	-5.28	1.17	1.24
1	E	15	HIS	CG-CD2	5.28	1.41	1.35
1	G	16	HIS	ND1-CE1	5.28	1.37	1.32
1	B	102	LYS	C-O	-5.28	1.17	1.24
1	D	217	ALA	C-O	5.26	1.30	1.23
1	E	144	LEU	CA-C	-5.26	1.46	1.52
1	A	87	PRO	N-CA	-5.25	1.41	1.46
1	G	204	TYR	C-O	-5.21	1.18	1.24
1	D	92	LYS	N-CA	-5.18	1.40	1.46
1	G	60	LYS	C-O	-5.16	1.17	1.24
1	D	50	HIS	CA-C	-5.16	1.45	1.52
1	G	15	HIS	ND1-CE1	5.14	1.37	1.32
1	B	93	LEU	N-CA	5.13	1.52	1.46
1	D	74	LEU	C-O	-5.11	1.18	1.24
1	B	189	HIS	CE1-NE2	5.10	1.37	1.32
1	B	164	ASN	C-O	-5.10	1.18	1.24
1	G	151	ARG	CA-C	-5.08	1.46	1.52
1	E	30	HIS	CG-ND1	-5.06	1.32	1.38
1	F	201	TRP	CD2-CE2	5.05	1.50	1.41
1	G	248	TRP	CD2-CE2	5.05	1.50	1.41
1	D	28	ASP	C-O	-5.04	1.18	1.24
1	B	16	HIS	CG-CD2	5.02	1.41	1.35
1	B	249	ARG	CZ-NH2	-5.00	1.26	1.33

All (74) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	249	ARG	NE-CZ-NH2	-10.09	110.12	119.20
1	G	249	ARG	NE-CZ-NH1	9.41	130.91	121.50
1	D	249	ARG	NE-CZ-NH2	-9.10	111.01	119.20
1	A	249	ARG	NE-CZ-NH2	-8.40	111.64	119.20
1	G	6	VAL	N-CA-CB	-8.23	99.35	110.54
1	E	6	VAL	N-CA-CB	-7.89	101.75	110.51
1	D	249	ARG	NE-CZ-NH1	7.46	128.97	121.50
1	F	290	GLY	N-CA-C	-7.14	97.78	112.34
1	F	249	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	B	139	ARG	N-CA-C	-6.61	105.13	113.72
1	G	290	GLY	N-CA-C	-6.54	99.00	112.34
1	D	6	VAL	N-CA-CB	-6.43	100.94	110.58
1	A	289	SER	CA-C-O	6.35	123.39	119.77
1	G	126	ALA	N-CA-C	-6.24	104.39	111.07
1	B	249	ARG	NE-CZ-NH2	-6.08	113.73	119.20
1	G	159	SER	CA-C-N	-5.99	115.38	122.93
1	G	159	SER	C-N-CA	-5.99	115.38	122.93
1	D	79	SER	CA-C-N	-5.97	112.76	121.71
1	D	79	SER	C-N-CA	-5.97	112.76	121.71
1	F	249	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	D	159	SER	CA-C-N	-5.88	115.52	122.93
1	D	159	SER	C-N-CA	-5.88	115.52	122.93
1	E	51	PHE	CA-C-N	-5.86	115.64	120.33
1	E	51	PHE	C-N-CA	-5.86	115.64	120.33
1	E	144	LEU	CA-C-N	-5.82	112.64	123.01
1	E	144	LEU	C-N-CA	-5.82	112.64	123.01
1	D	139	ARG	N-CA-C	-5.75	106.25	113.72
1	A	6	VAL	N-CA-C	-5.72	105.29	113.07
1	G	78	ASN	CA-CB-CG	-5.72	106.88	112.60
1	B	21	GLN	N-CA-C	-5.71	105.13	111.36
1	E	47	GLN	CB-CG-CD	-5.68	102.94	112.60
1	E	140	ALA	N-CA-C	-5.64	102.67	109.83
1	F	21	GLN	N-CA-C	-5.62	105.30	111.82
1	E	78	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	40	PHE	N-CA-CB	-5.61	101.59	110.22
1	G	262	GLY	N-CA-C	-5.55	106.06	112.50
1	D	290	GLY	N-CA-C	-5.55	101.03	112.34
1	G	242	LYS	O-C-N	5.53	125.69	121.65
1	B	33	MET	CA-CB-CG	-5.50	103.09	114.10
1	D	6	VAL	CB-CA-C	-5.50	104.63	112.22
1	B	40	PHE	N-CA-CB	-5.48	102.06	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	ARG	N-CA-C	-5.47	106.56	113.18
1	F	134	ARG	CA-CB-CG	-5.45	103.21	114.10
1	E	159	SER	CA-C-N	-5.44	116.07	122.93
1	E	159	SER	C-N-CA	-5.44	116.07	122.93
1	D	102	LYS	N-CA-C	-5.44	105.43	111.36
1	B	139	ARG	CG-CD-NE	-5.37	100.18	112.00
1	E	225	THR	N-CA-C	-5.36	105.43	111.28
1	F	245	GLY	N-CA-C	-5.32	102.47	111.08
1	G	121	LEU	N-CA-C	-5.29	105.60	111.36
1	A	47	GLN	CB-CG-CD	-5.28	103.62	112.60
1	F	68	ALA	N-CA-C	-5.28	105.60	111.36
1	E	6	VAL	CG1-CB-CG2	5.28	122.41	110.80
1	B	204	TYR	N-CA-C	-5.27	105.61	111.36
1	D	48	PHE	CA-C-N	-5.22	114.86	120.03
1	D	48	PHE	C-N-CA	-5.22	114.86	120.03
1	A	25	VAL	N-CA-C	-5.21	105.63	110.53
1	A	5	SER	CA-C-O	-5.20	115.84	121.87
1	B	159	SER	CA-C-N	-5.19	116.75	123.19
1	B	159	SER	C-N-CA	-5.19	116.75	123.19
1	F	249	ARG	CB-CG-CD	-5.19	99.37	111.30
1	F	69	GLU	N-CA-C	-5.16	105.73	111.36
1	E	6	VAL	CB-CA-C	-5.14	105.30	111.88
1	B	96	LEU	N-CA-C	-5.13	106.86	113.02
1	D	90	THR	CA-C-N	-5.12	113.65	119.28
1	D	90	THR	C-N-CA	-5.12	113.65	119.28
1	F	33	MET	CA-CB-CG	-5.10	103.90	114.10
1	D	30	HIS	CB-CA-C	-5.08	102.69	110.81
1	B	274	ILE	CG1-CB-CG2	-5.07	95.49	110.70
1	F	159	SER	CA-C-N	-5.07	116.55	122.93
1	F	159	SER	C-N-CA	-5.07	116.55	122.93
1	G	249	ARG	CD-NE-CZ	5.05	131.47	124.40
1	D	78	ASN	CA-CB-CG	-5.01	107.59	112.60
1	E	40	PHE	N-CA-CB	-5.01	102.76	110.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2399	0	2398	28	0
1	B	2388	0	2380	27	0
1	D	2388	0	2375	25	0
1	E	2391	0	2385	35	0
1	F	2405	0	2404	33	0
1	G	2411	0	2414	36	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	175	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 (175) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:289[A]:SER:CA	3:F:719:HOH:O	2.25	0.78
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:29:ILE:HD13	1:F:42:ILE:HD13	1.93	0.50
1:F:142:GLN:H	1:F:142:GLN:NE2	2.09	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
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:B:95:ARG:HA	1:G:147:ARG:NH1	2.30	0.47
1:E:169:GLU:HG3	3:E:728:HOH:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:G:52:ILE:HA	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:F:4:ARG:HG2	1:F:5:SER:N	2.25	0.45
1:G:205:LEU:HD23	1:G:205:LEU:HA	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:H	1:E:16:HIS:CD2	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:HD13	1:D:52:ILE:HA	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:OD2	1:D:194:ASP:N	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:49:PRO:HB2	1:E:50:HIS:CD2	2.53	0.43
1:E:194:ASP:OD2	1:E:194:ASP:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:THR:HG23	1:G:228:ARG:NH2	2.34	0.42
1:D:41:GLY:HA2	1:D:270:TYR:CZ	2.54	0.42
1:D:208:ALA:HB1	1:D:284:LEU:HD22	2.01	0.42
1:B:215:PRO:HG3	2:B:402:GOL:H31	2.02	0.42
1:G:268:PHE:CD2	1:G:268:PHE:C	2.98	0.42
1:B:158:ASN:H	1:B:158:ASN:ND2	2.17	0.42
1:D:4:ARG:NH1	1:E:250:ASP:OD1	2.41	0.42
1:D:29:ILE:HD13	1:D:42:ILE:HD13	2.01	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:HA	1:E:74:LEU:HD12	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:A:74:LEU:HD23	1:A:74:LEU:HA	1.91	0.41
1:F:131:TRP:CD2	1:F:248:TRP:HB3	2.55	0.41
1:G:180:ARG:HD2	1:G:180:ARG:C	2.45	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:31:ASN:HD22	1:D:155:GLY:HA2	1.87	0.40
1:D:285:LYS:HE2	3:D:693:HOH:O	2.22	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:E:268:PHE:CD2	1:E:268:PHE:C	3.00	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%)	84	80
1	B	250/251 (100%)	248 (99%)	2 (1%)	73	65
1	D	250/251 (100%)	247 (99%)	3 (1%)	63	51
1	E	251/251 (100%)	248 (99%)	3 (1%)	63	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	253/251 (101%)	248 (98%)	5 (2%)	48	32
1	G	255/251 (102%)	254 (100%)	1 (0%)	84	80
All	All	1511/1506 (100%)	1496 (99%)	15 (1%)	68	58

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	19	LYS
1	D	14	ASP
1	D	19	LYS
1	D	242	LYS
1	E	53	PRO
1	E	118	PRO
1	E	253	GLU
1	F	14	ASP
1	F	74	LEU
1	F	142	GLN
1	F	158	ASN
1	F	169	GLU
1	G	14	ASP

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

Mol	Chain	Res	Type
1	A	16	HIS
1	B	16	HIS
1	B	31	ASN
1	B	158	ASN
1	D	16	HIS
1	D	31	ASN
1	D	47	GLN
1	D	117	ASN
1	D	158	ASN
1	E	16	HIS
1	E	117	ASN
1	E	176	GLN
1	E	271	ASN
1	F	16	HIS

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Mol	Chain	Res	Type
1	F	31	ASN
1	F	62	ASN
1	F	142	GLN
1	G	16	HIS
1	G	31	ASN
1	G	142	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	401	-	5,5,5	0.73	0	5,5,5	1.14	1 (20%)
2	GOL	E	402	-	5,5,5	0.68	0	5,5,5	0.94	0
2	GOL	G	402	-	5,5,5	0.82	0	5,5,5	1.28	1 (20%)
2	GOL	F	401	-	5,5,5	0.82	0	5,5,5	0.70	0
2	GOL	B	402	-	5,5,5	1.04	0	5,5,5	1.48	0
2	GOL	E	401	-	5,5,5	0.95	0	5,5,5	1.08	0
2	GOL	A	402	-	5,5,5	0.64	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	402	-	5,5,5	0.45	0	5,5,5	0.97	0
2	GOL	D	401	-	5,5,5	0.88	0	5,5,5	0.69	0
2	GOL	A	401	-	5,5,5	0.81	0	5,5,5	0.60	0
2	GOL	F	402	-	5,5,5	0.82	0	5,5,5	0.93	0
2	GOL	B	401	-	5,5,5	1.07	0	5,5,5	0.82	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	G	401	-	-	0/4/4/4	-
2	GOL	E	402	-	-	0/4/4/4	-
2	GOL	G	402	-	-	2/4/4/4	-
2	GOL	F	401	-	-	0/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	E	401	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	D	402	-	-	0/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	F	402	-	-	0/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	GOL	O3-C3-C2	-2.14	100.74	110.38
2	G	402	GOL	O1-C1-C2	-2.09	100.97	110.38

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	298/301 (99%)	-0.80	1 (0%)	90	91	5, 9, 23, 40	4 (1%)
1	B	298/301 (99%)	-0.77	3 (1%)	79	82	5, 9, 24, 42	4 (1%)
1	D	298/301 (99%)	-0.82	1 (0%)	90	91	5, 8, 22, 49	2 (0%)
1	E	298/301 (99%)	-0.81	3 (1%)	79	82	4, 8, 22, 46	2 (0%)
1	F	298/301 (99%)	-0.78	1 (0%)	90	91	5, 9, 25, 52	4 (1%)
1	G	298/301 (99%)	-0.76	4 (1%)	75	79	5, 9, 23, 48	6 (2%)
All	All	1788/1806 (99%)	-0.79	13 (0%)	84	86	4, 9, 23, 52	22 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	141	PRO	4.8
1	B	141	PRO	3.4
1	E	141	PRO	3.2
1	G	141	PRO	3.1
1	A	141	PRO	2.7
1	D	140	ALA	2.6
1	G	158	ASN	2.3
1	B	158	ASN	2.3
1	G	6	VAL	2.1
1	B	8	GLY	2.1
1	E	145	ARG	2.1
1	G	142	GLN	2.1
1	E	158	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	GOL	E	401	6/6	0.93	0.11	14,19,22,24	0
2	GOL	F	401	6/6	0.93	0.11	18,23,25,29	0
2	GOL	D	401	6/6	0.94	0.09	14,19,22,27	0
2	GOL	A	401	6/6	0.94	0.10	16,21,21,27	0
2	GOL	B	401	6/6	0.94	0.09	16,23,24,24	0
2	GOL	G	401	6/6	0.94	0.10	19,22,24,28	0
2	GOL	F	402	6/6	0.96	0.09	13,18,19,22	0
2	GOL	B	402	6/6	0.96	0.08	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	0.06	12,15,15,19	0
2	GOL	A	402	6/6	0.98	0.05	13,15,16,17	0
2	GOL	E	402	6/6	0.99	0.04	13,15,15,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.