



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:50 AM UTC

PDB ID : 4KEU / pdb_00004keu
Title : Crystal structure of SsoPox W263M
Authors : Gotthard, G.; Hiblot, J.; Chabriere, E.; Elias, M.
Deposited on : 2013-04-26
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

<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

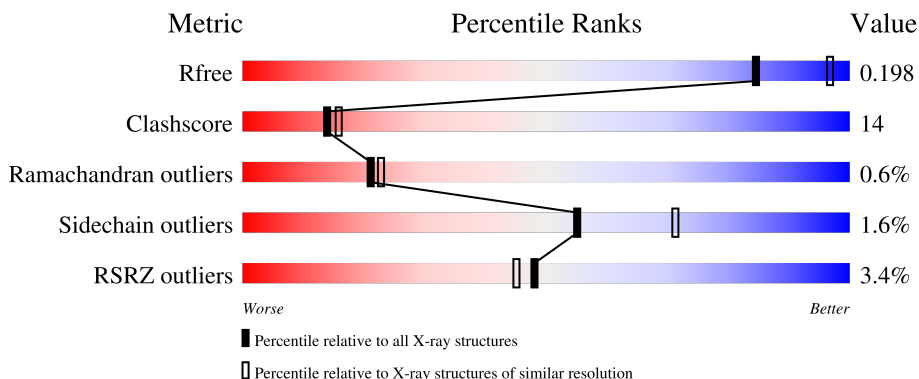
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	314	4% 75% 24% .
1	B	314	3% 70% 27% .
1	C	314	2% 73% 25% .
1	D	314	4% 69% 27% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10557 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 Aryldialkylphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	4	0
			2548	1632	435	472	9			
1	B	314	Total	C	N	O	S	0	3	0
			2534	1625	430	470	9			
1	C	314	Total	C	N	O	S	0	3	0
			2531	1625	429	469	8			
1	D	314	Total	C	N	O	S	0	4	0
			2548	1633	435	472	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	MET	TRP	engineered mutation	UNP Q97VT7
B	263	MET	TRP	engineered mutation	UNP Q97VT7
C	263	MET	TRP	engineered mutation	UNP Q97VT7
D	263	MET	TRP	engineered mutation	UNP Q97VT7

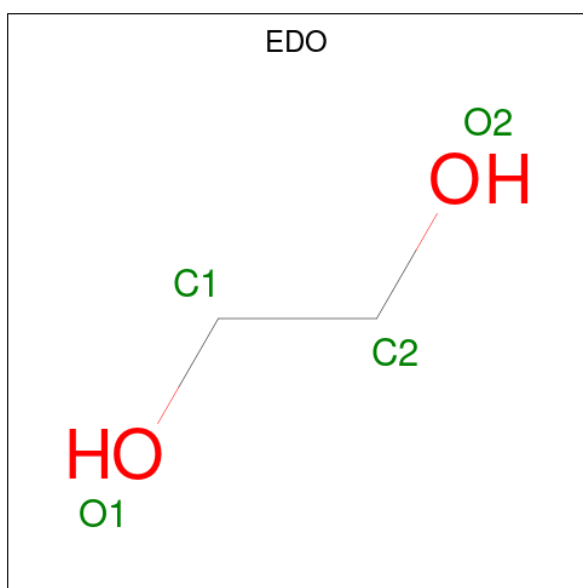
- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co 1 1	0	0
3	B	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0
3	D	1	Total Co 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

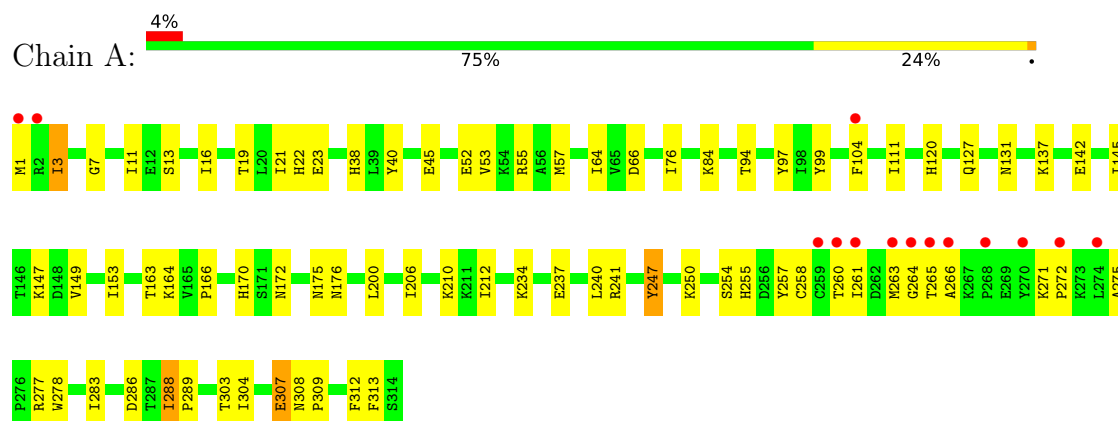
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	88	Total	O	0	0
			88	88		
6	B	86	Total	O	0	0
			86	86		
6	C	74	Total	O	0	0
			74	74		
6	D	84	Total	O	0	0
			84	84		

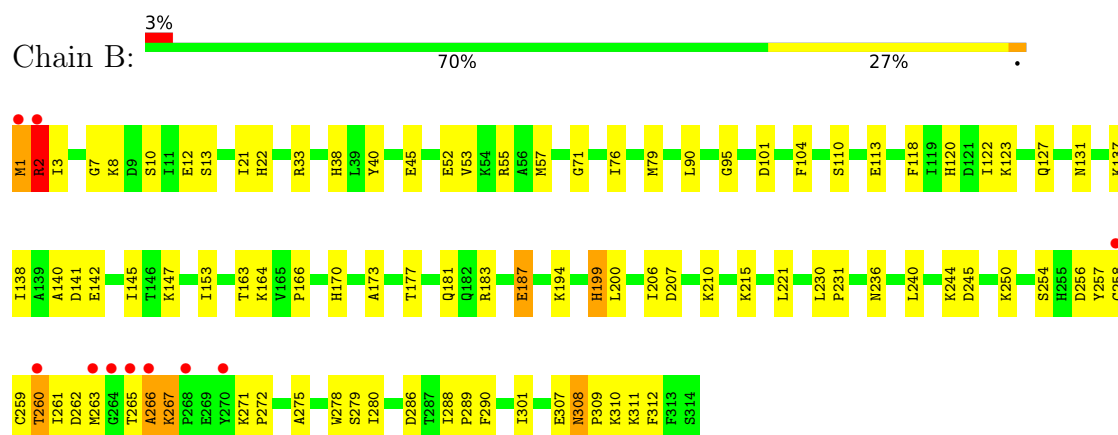
3 Residue-property plots

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.

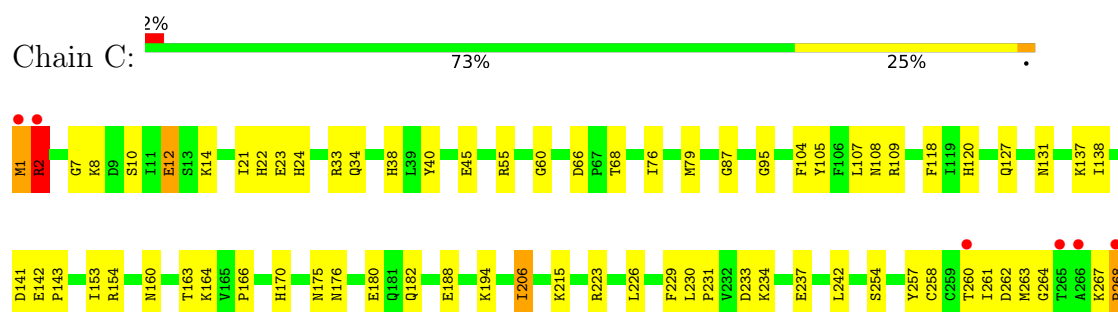
• Molecule 1: Aryldialkylphosphatase

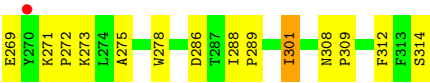


• Molecule 1: Aryldialkylphosphatase

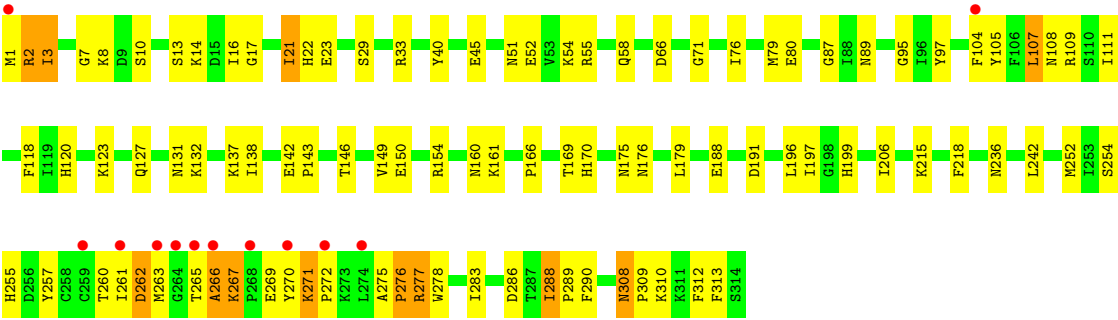


• Molecule 1: Aryldialkylphosphatase





● Molecule 1: Aryldialkylphosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.82Å 103.88Å 151.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.20 49.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.14-2.20) 99.9 (49.14-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.215 (Not available) , 0.198	Depositor DCC
R_{free} test set	3511 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10557	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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: KCX, GOL, FE2, CO, EDO

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	23/2585 (0.9%)	0.69	1/3486 (0.0%)
1	B	1.51	22/2574 (0.9%)	0.69	1/3472 (0.0%)
1	C	1.44	12/2574 (0.5%)	0.68	0/3473
1	D	1.47	19/2585 (0.7%)	0.70	0/3487
All	All	1.48	76/10318 (0.7%)	0.69	2/13918 (0.0%)

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	ILE	N-CA	10.38	1.54	1.46
1	A	288	ILE	CA-C	9.65	1.61	1.52
1	A	111	ILE	N-CA	-7.21	1.38	1.46
1	A	3	ILE	N-CA	6.97	1.51	1.46
1	C	170	HIS	CG-CD2	6.73	1.43	1.35
1	D	170	HIS	N-CA	-6.71	1.38	1.46
1	C	14	LYS	C-O	-6.62	1.15	1.24
1	B	140	ALA	CA-C	-6.53	1.44	1.52
1	A	38	HIS	CG-CD2	6.48	1.43	1.35
1	A	170	HIS	CG-CD2	6.47	1.43	1.35
1	C	21	ILE	CA-C	6.45	1.60	1.52
1	D	120	HIS	CG-CD2	6.33	1.42	1.35
1	D	308	ASN	C-O	-6.23	1.18	1.24
1	A	247	TYR	N-CA	6.19	1.53	1.46
1	B	280	ILE	CA-C	6.17	1.59	1.52
1	B	147	LYS	C-O	-6.14	1.17	1.24
1	A	22	HIS	CB-CG	6.05	1.58	1.50
1	D	22	HIS	CG-CD2	6.04	1.42	1.35
1	B	22	HIS	CG-CD2	5.99	1.42	1.35
1	C	24	HIS	CG-CD2	5.89	1.42	1.35
1	B	170	HIS	CG-CD2	5.87	1.42	1.35
1	B	123	LYS	N-CA	5.86	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	34	GLN	CA-C	5.79	1.60	1.52
1	B	199	HIS	CG-CD2	5.72	1.42	1.35
1	D	80	GLU	N-CA	5.69	1.53	1.46
1	A	170	HIS	N-CA	-5.69	1.39	1.46
1	A	120	HIS	CG-CD2	5.66	1.42	1.35
1	D	21	ILE	CA-C	5.63	1.58	1.52
1	A	40	TYR	CA-C	-5.49	1.46	1.52
1	C	24	HIS	ND1-CE1	5.47	1.38	1.32
1	B	170	HIS	N-CA	-5.46	1.39	1.46
1	C	170	HIS	CE1-NE2	5.45	1.38	1.32
1	B	187	GLU	N-CA	5.43	1.53	1.46
1	A	22	HIS	CG-CD2	5.39	1.41	1.35
1	A	170	HIS	CE1-NE2	5.38	1.38	1.32
1	A	240	LEU	CA-C	5.38	1.59	1.52
1	D	170	HIS	CG-CD2	5.37	1.41	1.35
1	C	12	GLU	N-CA	-5.36	1.39	1.46
1	B	250	LYS	N-CA	5.36	1.52	1.45
1	D	111	ILE	N-CA	-5.35	1.40	1.46
1	A	64	ILE	N-CA	-5.35	1.40	1.46
1	A	212	ILE	C-O	5.31	1.30	1.24
1	B	199	HIS	ND1-CE1	5.31	1.37	1.32
1	C	206	ILE	CA-C	5.30	1.59	1.52
1	D	288	ILE	CA-C	5.30	1.57	1.52
1	B	308	ASN	C-O	-5.28	1.19	1.24
1	B	8	LYS	CA-C	-5.27	1.46	1.52
1	C	60	GLY	CA-C	5.26	1.59	1.51
1	B	215	LYS	C-O	-5.26	1.17	1.24
1	C	120	HIS	CG-CD2	5.25	1.41	1.35
1	B	221	LEU	CA-C	-5.24	1.47	1.53
1	A	22	HIS	CA-CB	5.23	1.59	1.52
1	D	199	HIS	CG-CD2	5.21	1.41	1.35
1	A	21	ILE	CA-C	5.19	1.60	1.52
1	A	94	THR	N-CA	-5.18	1.38	1.46
1	B	122	ILE	CA-C	5.16	1.59	1.52
1	D	3	ILE	N-CA	5.16	1.51	1.46
1	D	22	HIS	ND1-CE1	5.16	1.37	1.32
1	D	89	ASN	CA-C	-5.14	1.46	1.52
1	D	97	TYR	CA-C	5.14	1.59	1.53
1	A	172	ASN	N-CA	-5.13	1.39	1.46
1	A	142	GLU	N-CA	5.12	1.51	1.46
1	A	84	LYS	C-O	-5.11	1.17	1.24
1	B	22	HIS	CE1-NE2	5.08	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	276	PRO	CA-C	5.07	1.59	1.52
1	B	38	HIS	CG-CD2	5.07	1.41	1.35
1	D	271	LYS	CA-C	5.06	1.58	1.52
1	B	256	ASP	CB-CG	5.06	1.64	1.52
1	B	120	HIS	CG-CD2	5.04	1.41	1.35
1	D	262	ASP	CA-C	5.03	1.59	1.52
1	A	307	GLU	C-O	-5.02	1.18	1.24
1	D	199	HIS	ND1-CE1	5.02	1.37	1.32
1	A	304	ILE	CA-C	5.01	1.59	1.52
1	C	22	HIS	ND1-CE1	5.01	1.37	1.32
1	B	21	ILE	CA-C	5.01	1.58	1.52
1	D	197	ILE	CA-C	5.00	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ILE	N-CA-C	5.62	112.22	106.21
1	A	145	ILE	N-CA-C	5.14	111.71	106.21

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	2548	0	2583	58	0
1	B	2534	0	2572	69	0
1	C	2531	0	2572	70	0
1	D	2548	0	2582	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	8	0	12	2	0
4	B	4	0	6	0	0
4	D	8	0	12	0	0
5	A	12	0	16	0	0
5	B	6	0	8	2	0
5	C	6	0	8	1	0
5	D	12	0	16	2	0
6	A	88	0	0	6	0
6	B	86	0	0	3	0
6	C	74	0	0	3	0
6	D	84	0	0	3	0
All	All	10557	0	10387	297	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 14.

All (297) 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:A:265:THR:HG22	1:C:108:ASN:ND2	1.26	1.37
1:D:2[B]:ARG:NH2	1:D:2[B]:ARG:HA	1.55	1.21
1:A:265:THR:CG2	1:C:108:ASN:ND2	2.13	1.11
1:D:277[B]:ARG:HG2	1:D:277[B]:ARG:HH11	1.00	1.08
1:C:2[A]:ARG:HH11	1:C:2[A]:ARG:CG	1.62	1.08
1:A:277[B]:ARG:HH11	1:A:277[B]:ARG:HG2	1.04	1.07
1:D:2[B]:ARG:HG2	1:D:2[B]:ARG:HH21	1.12	1.07
1:D:2[B]:ARG:HH21	1:D:2[B]:ARG:CG	1.64	1.07
1:B:263:MET:HE2	1:B:265:THR:HB	1.34	1.06
1:D:2[A]:ARG:CG	1:D:2[A]:ARG:HH21	1.64	1.06
1:A:265:THR:CG2	1:C:108:ASN:HD22	1.69	1.06
1:D:277[A]:ARG:HH11	1:D:277[A]:ARG:CG	1.68	1.06
1:D:277[A]:ARG:HH11	1:D:277[A]:ARG:HG2	1.13	1.04
1:D:16[A]:ILE:HD12	1:D:17:GLY:N	1.72	1.04
1:D:277[B]:ARG:HH11	1:D:277[B]:ARG:CG	1.71	1.02
1:D:261:ILE:HD11	1:D:263:MET:CE	1.92	1.00
1:B:206:ILE:HD12	1:B:207:ASP:N	1.75	1.00
1:A:277[B]:ARG:HH11	1:A:277[B]:ARG:CG	1.73	0.99
1:D:206:ILE:HD11	1:D:242:LEU:CD2	1.92	0.99
1:A:265:THR:HG22	1:C:108:ASN:HD21	1.27	0.98
1:B:2[B]:ARG:HH21	1:B:2[B]:ARG:HB3	1.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2[A]:ARG:HH11	1:C:2[A]:ARG:HG2	1.28	0.97
1:B:271:LYS:HB3	1:B:272:PRO:HD3	1.49	0.95
1:D:261:ILE:HD11	1:D:263:MET:HE1	1.51	0.92
1:D:277[B]:ARG:HG2	1:D:277[B]:ARG:NH1	1.82	0.92
1:D:2[B]:ARG:NH2	1:D:2[B]:ARG:HG2	1.82	0.91
1:B:52:GLU:OE1	1:B:55:ARG:NH2	2.04	0.91
1:D:2[B]:ARG:NH2	1:D:2[B]:ARG:CA	2.34	0.89
1:D:2[B]:ARG:HA	1:D:2[B]:ARG:CZ	2.03	0.89
1:D:2[A]:ARG:HH21	1:D:2[A]:ARG:HG2	1.35	0.88
1:B:1[B]:MET:SD	1:B:1[B]:MET:N	2.46	0.88
1:A:263:MET:HG2	1:C:104[A]:PHE:HD2	1.39	0.87
1:D:2[A]:ARG:HH21	1:D:2[A]:ARG:HG3	1.39	0.86
1:B:1[B]:MET:HE2	1:B:12:GLU:HG3	1.58	0.85
1:D:277[A]:ARG:HG2	1:D:277[A]:ARG:NH1	1.90	0.85
1:A:277[B]:ARG:HG2	1:A:277[B]:ARG:NH1	1.84	0.85
1:C:2[A]:ARG:HH11	1:C:2[A]:ARG:HG3	1.41	0.84
1:C:107:LEU:HD22	6:C:554:HOH:O	1.79	0.82
1:C:2[A]:ARG:CG	1:C:2[A]:ARG:NH1	2.34	0.82
1:D:206:ILE:HD11	1:D:242:LEU:CG	2.10	0.81
1:A:265:THR:HG22	1:C:108:ASN:HD22	0.98	0.80
1:D:2[B]:ARG:HH21	1:D:2[B]:ARG:CB	1.93	0.80
1:D:276:PRO:HB2	1:D:277[B]:ARG:HD3	1.62	0.79
1:D:206:ILE:HD11	1:D:242:LEU:HG	1.63	0.78
1:A:104[B]:PHE:HE2	1:C:262:ASP:OD1	1.65	0.78
1:B:1[A]:MET:SD	1:B:1[A]:MET:N	2.57	0.78
1:B:1[A]:MET:HE2	1:B:12:GLU:HG3	1.64	0.78
1:D:2[A]:ARG:CG	1:D:2[A]:ARG:NH2	2.37	0.77
1:A:275:ALA:HB1	1:A:278:TRP:HB2	1.68	0.76
1:D:107:LEU:O	1:D:108:ASN:HB2	1.87	0.74
1:C:206:ILE:HD11	1:C:242:LEU:HG	1.70	0.72
1:D:206:ILE:HD11	1:D:242:LEU:HD21	1.70	0.72
1:A:271:LYS:HB3	1:A:272:PRO:HD3	1.71	0.71
1:C:2[A]:ARG:HG2	1:C:2[A]:ARG:NH1	1.99	0.71
1:B:230:LEU:HD12	1:B:231:PRO:HD2	1.73	0.71
1:D:196:LEU:HD22	1:D:252:MET:HE3	1.71	0.70
1:D:161:LYS:CE	1:D:188:GLU:O	2.40	0.70
1:B:194:LYS:HG3	5:B:404:GOL:H11	1.71	0.69
1:D:45:GLU:HG2	1:D:260:THR:HG21	1.73	0.69
1:A:52:GLU:OE1	1:A:55:ARG:NH2	2.26	0.68
1:B:206:ILE:HD12	1:B:207:ASP:H	1.58	0.68
1:B:257:TYR:HA	1:B:278:TRP:CZ2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2[B]:ARG:NH2	1:D:2[B]:ARG:CG	2.37	0.68
1:D:277[B]:ARG:HD3	1:D:277[B]:ARG:N	2.08	0.68
1:D:13:SER:O	1:D:16[A]:ILE:HG13	1.94	0.67
1:C:154:ARG:NH2	1:C:188:GLU:OE2	2.28	0.67
1:A:1[B]:MET:SD	1:A:1[B]:MET:N	2.65	0.67
1:D:160:ASN:OD1	5:D:405:GOL:H2	1.94	0.66
1:A:261:ILE:HG23	1:A:266:ALA:CB	2.25	0.66
1:A:263:MET:CG	1:C:104[A]:PHE:HD2	2.06	0.66
1:C:1:MET:SD	1:C:1:MET:N	2.69	0.66
1:A:16:ILE:HG22	1:A:19:THR:OG1	1.95	0.66
1:D:263:MET:HB3	1:D:265:THR:HG22	1.78	0.66
1:A:234:LYS:O	1:A:237:GLU:HG2	1.97	0.65
1:C:55:ARG:HD3	6:C:538:HOH:O	1.96	0.65
1:B:76:ILE:H	1:B:127:GLN:HE22	1.44	0.64
1:B:7:GLY:H	1:B:131:ASN:ND2	1.95	0.64
1:C:273:LYS:HD2	1:C:273:LYS:N	2.12	0.64
1:A:277[B]:ARG:CG	1:A:277[B]:ARG:NH1	2.44	0.63
1:D:7:GLY:H	1:D:131:ASN:ND2	1.96	0.63
1:D:206:ILE:CD1	1:D:242:LEU:HG	2.28	0.63
1:D:266:ALA:O	1:D:267:LYS:O	2.16	0.63
1:D:161:LYS:HE3	1:D:188:GLU:O	1.97	0.63
1:B:266:ALA:O	1:B:267:LYS:O	2.16	0.63
1:A:76:ILE:H	1:A:127:GLN:HE22	1.45	0.63
1:B:240:LEU:HG	1:B:244:LYS:HE2	1.81	0.63
1:B:2[B]:ARG:HH21	1:B:2[B]:ARG:CB	2.08	0.62
1:A:250:LYS:HE3	6:A:547:HOH:O	1.98	0.62
1:D:2[A]:ARG:HG2	1:D:2[A]:ARG:NH2	2.10	0.62
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.34	0.62
1:D:206:ILE:CD1	1:D:242:LEU:HD21	2.29	0.62
1:D:1:MET:HG3	1:D:10:SER:O	1.99	0.61
1:C:2[A]:ARG:HG3	1:C:2[A]:ARG:NH1	2.10	0.61
1:D:2[A]:ARG:HG3	1:D:2[A]:ARG:NH2	2.06	0.61
1:D:138:ILE:C	1:D:138:ILE:HD12	2.26	0.60
1:B:2[B]:ARG:HB3	1:B:2[B]:ARG:NH2	2.10	0.60
1:D:2[B]:ARG:CA	1:D:2[B]:ARG:CZ	2.77	0.60
5:B:404:GOL:H12	6:B:574:HOH:O	2.02	0.60
1:C:275:ALA:HB1	1:C:278:TRP:HB2	1.84	0.60
1:B:76:ILE:H	1:B:127:GLN:NE2	1.99	0.60
1:C:233:ASP:O	1:C:237:GLU:HG3	2.02	0.60
1:D:196:LEU:HD22	1:D:252:MET:CE	2.32	0.59
1:D:16[A]:ILE:HD12	1:D:16[A]:ILE:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277[B]:ARG:CG	1:D:277[B]:ARG:NH1	2.41	0.58
1:C:264:GLY:O	1:C:267:LYS:HG2	2.03	0.58
1:B:138:ILE:HD12	1:B:153:ILE:HG12	1.85	0.58
1:D:257:TYR:HA	1:D:278:TRP:CZ2	2.39	0.58
1:C:7:GLY:H	1:C:131:ASN:ND2	2.02	0.58
1:D:275:ALA:HB1	1:D:278:TRP:HB2	1.86	0.57
1:B:262:ASP:OD1	1:D:104[B]:PHE:HE1	1.87	0.57
1:C:163:THR:O	1:C:164:LYS:HB2	2.04	0.57
1:B:275:ALA:HB1	1:B:278:TRP:HB2	1.87	0.57
1:D:206:ILE:CD1	1:D:242:LEU:CD2	2.77	0.57
1:B:271:LYS:HB3	1:B:272:PRO:CD	2.30	0.57
1:D:236:ASN:HB3	1:D:290:PHE:CE2	2.40	0.57
1:D:52:GLU:OE1	1:D:55:ARG:NH2	2.37	0.57
1:B:1[A]:MET:O	1:B:2[A]:ARG:HB2	2.04	0.56
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.40	0.56
1:D:2[B]:ARG:NH2	1:D:2[B]:ARG:CB	2.62	0.56
1:D:79:MET:HE3	6:D:514:HOH:O	2.05	0.56
1:B:206:ILE:HD12	1:B:206:ILE:C	2.28	0.56
1:C:206:ILE:HD11	1:C:242:LEU:CD2	2.35	0.56
1:D:2[B]:ARG:O	1:D:2[B]:ARG:NE	2.37	0.56
1:B:307:GLU:HG3	1:B:311:LYS:NZ	2.20	0.56
1:D:76:ILE:H	1:D:127:GLN:NE2	2.03	0.56
1:D:3:ILE:HD11	1:D:313:PHE:HB3	1.88	0.56
1:C:206:ILE:HD11	1:C:242:LEU:CG	2.36	0.55
1:A:263:MET:CG	1:C:104[A]:PHE:CD2	2.88	0.55
1:A:76:ILE:H	1:A:127:GLN:NE2	2.03	0.55
1:B:311:LYS:HE2	6:B:545:HOH:O	2.06	0.55
1:A:308:ASN:HB2	1:A:309:PRO:HD3	1.89	0.55
1:A:263:MET:HG2	1:C:104[A]:PHE:CD2	2.31	0.55
1:B:259:CYS:O	1:B:260:THR:HG23	2.07	0.54
1:B:79:MET:HE2	1:B:90:LEU:HD21	1.87	0.54
1:C:261:ILE:HG12	1:C:263:MET:HG2	1.88	0.54
1:A:286:ASP:OD1	1:A:286:ASP:C	2.50	0.54
1:D:54:LYS:O	1:D:58:GLN:HG3	2.07	0.54
1:D:76:ILE:H	1:D:127:GLN:HE22	1.56	0.54
1:B:261:ILE:HG12	1:B:263:MET:HG2	1.88	0.54
1:C:45:GLU:HG2	1:C:260:THR:HG21	1.90	0.53
1:C:288:ILE:HB	1:C:289:PRO:HD3	1.91	0.53
1:D:261:ILE:HD11	1:D:263:MET:HE2	1.86	0.53
1:A:206:ILE:HD13	1:A:241:ARG:HG2	1.89	0.53
1:A:277[B]:ARG:HH11	1:A:277[B]:ARG:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:GLU:OE2	1:C:180:GLU:HA	2.08	0.53
1:D:105:TYR:O	1:D:109:ARG:NH1	2.41	0.53
1:B:45:GLU:HA	1:B:260:THR:HG21	1.90	0.52
1:A:52:GLU:CD	1:A:55:ARG:HH22	2.17	0.52
1:C:141:ASP:OD1	1:C:142:GLU:N	2.39	0.52
1:B:104[B]:PHE:HE2	1:D:71:GLY:O	1.91	0.52
1:B:288:ILE:HB	1:B:289:PRO:HD3	1.92	0.52
1:D:277[A]:ARG:CG	1:D:277[A]:ARG:NH1	2.41	0.52
1:C:1:MET:HA	1:C:10:SER:OG	2.09	0.52
1:D:261:ILE:CD1	1:D:263:MET:CE	2.78	0.52
1:A:13:SER:O	1:A:16:ILE:HG12	2.09	0.52
1:C:1:MET:O	1:C:2[A]:ARG:HB2	2.09	0.52
1:A:11:ILE:HD11	1:A:16:ILE:HD13	1.93	0.51
1:B:53:VAL:O	1:B:57:MET:HG3	2.10	0.51
1:B:2[B]:ARG:NH2	1:B:13:SER:H	2.08	0.51
1:B:101:ASP:HB2	6:B:548:HOH:O	2.10	0.51
1:A:45:GLU:HG2	1:A:260:THR:HG21	1.92	0.51
1:A:275:ALA:HB1	1:A:278:TRP:CB	2.40	0.50
1:C:95:GLY:HA2	1:C:118:PHE:CE1	2.45	0.50
1:B:104[B]:PHE:HE1	1:D:262:ASP:OD1	1.95	0.50
1:C:175:ASN:O	1:C:176:ASN:HB2	2.11	0.50
1:D:161:LYS:NZ	1:D:188:GLU:O	2.45	0.50
1:C:76:ILE:H	1:C:127:GLN:NE2	2.10	0.50
1:D:51:ASN:HA	1:D:54:LYS:HG2	1.93	0.50
1:D:166:PRO:HB2	1:D:312:PHE:CZ	2.47	0.50
1:A:176:ASN:HB3	6:A:564:HOH:O	2.11	0.50
1:D:218:PHE:CB	1:D:252:MET:HE2	2.42	0.50
1:D:271:LYS:N	1:D:272:PRO:HD2	2.27	0.50
1:B:307:GLU:HG3	1:B:311:LYS:HZ3	1.75	0.50
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.46	0.49
1:C:79:MET:HE3	6:C:510:HOH:O	2.11	0.49
1:A:175:ASN:O	1:A:176:ASN:CB	2.59	0.49
1:D:3:ILE:CD1	1:D:313:PHE:HB3	2.42	0.49
1:A:97:TYR:HH	1:A:99:TYR:HH	1.57	0.49
1:A:277[B]:ARG:NH1	1:A:277[B]:ARG:CB	2.76	0.49
1:D:277[B]:ARG:NH1	1:D:277[B]:ARG:CB	2.75	0.49
4:A:403:EDO:H11	6:A:530:HOH:O	2.12	0.49
1:A:258:CYS:C	1:A:260:THR:N	2.70	0.49
1:A:147:LYS:HG2	6:A:521:HOH:O	2.13	0.48
1:B:7:GLY:H	1:B:131:ASN:HD21	1.59	0.48
1:B:258:CYS:C	1:B:260:THR:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2[B]:ARG:HD3	1:D:3:ILE:HD13	1.94	0.48
1:D:277[B]:ARG:HH11	1:D:277[B]:ARG:CB	2.24	0.48
1:B:141:ASP:OD1	1:B:142:GLU:N	2.44	0.48
1:C:160:ASN:OD1	5:C:403:GOL:H2	2.14	0.48
1:C:267:LYS:HB2	1:C:268:PRO:HD2	1.96	0.48
1:D:175:ASN:O	1:D:176:ASN:HB3	2.14	0.48
1:D:218:PHE:HB3	1:D:252:MET:HE2	1.94	0.48
1:B:110:SER:OG	1:B:113:GLU:HG3	2.13	0.48
1:C:286:ASP:OD1	1:C:286:ASP:C	2.56	0.48
1:A:53:VAL:O	1:A:57:MET:HG3	2.13	0.48
1:A:163:THR:O	1:A:164:LYS:HB2	2.12	0.48
1:B:210:LYS:NZ	1:B:245:ASP:OD1	2.29	0.48
1:D:266:ALA:O	1:D:270:TYR:HB2	2.13	0.48
1:D:277[A]:ARG:HH11	1:D:277[A]:ARG:HG3	1.69	0.48
1:B:104[B]:PHE:CD1	1:D:263:MET:SD	3.06	0.48
1:A:255:HIS:NE2	1:A:283:ILE:HG23	2.28	0.47
1:B:183:ARG:HD2	1:B:187:GLU:OE1	2.14	0.47
1:C:138:ILE:HD12	1:C:153:ILE:HG12	1.96	0.47
1:B:236:ASN:HB3	1:B:290:PHE:CE2	2.50	0.47
1:D:276:PRO:HB2	1:D:277[B]:ARG:CD	2.40	0.47
1:D:286:ASP:C	1:D:286:ASP:OD1	2.57	0.47
1:C:269:GLU:H	1:C:269:GLU:CD	2.23	0.47
1:B:310:LYS:HB2	1:B:310:LYS:HE3	1.70	0.47
1:B:33:ARG:HA	1:B:40:TYR:CE1	2.50	0.46
1:D:123:LYS:O	1:D:132:LYS:HE3	2.15	0.46
1:C:66:ASP:OD1	1:C:68:THR:OG1	2.31	0.46
1:A:7:GLY:H	1:A:131:ASN:ND2	2.12	0.46
1:A:3:ILE:HD11	1:A:313:PHE:HB3	1.97	0.46
1:C:258:CYS:SG	1:C:261:ILE:HD12	2.55	0.46
1:B:275:ALA:HB1	1:B:278:TRP:CB	2.45	0.46
1:B:206:ILE:C	1:B:206:ILE:CD1	2.89	0.45
1:D:23:GLU:O	1:D:66:ASP:HA	2.16	0.45
1:A:3:ILE:CD1	1:A:313:PHE:HB3	2.45	0.45
1:C:7:GLY:H	1:C:131:ASN:HD21	1.63	0.45
1:A:66:ASP:OD1	1:A:66:ASP:C	2.60	0.45
1:A:210:LYS:HE2	1:A:247:TYR:CE1	2.50	0.45
1:B:257:TYR:CD2	1:B:279:SER:HA	2.52	0.45
1:B:183:ARG:CD	1:B:187:GLU:OE1	2.65	0.45
1:C:76:ILE:H	1:C:127:GLN:HE22	1.64	0.45
1:D:16[A]:ILE:HD13	1:D:17:GLY:O	2.17	0.45
1:D:308:ASN:HB2	1:D:309:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:TYR:CE2	1:B:279:SER:HA	2.52	0.45
1:C:257:TYR:HA	1:C:278:TRP:CZ2	2.52	0.45
1:A:104[B]:PHE:C	1:A:104[B]:PHE:CD2	2.95	0.44
1:C:308:ASN:HB2	1:C:309:PRO:HD3	1.97	0.44
1:C:142:GLU:HB3	1:C:143:PRO:HD3	1.98	0.44
1:C:182:GLN:NE2	1:C:215:LYS:HB2	2.32	0.44
1:B:52:GLU:CD	1:B:55:ARG:HH22	2.15	0.44
1:D:33:ARG:HA	1:D:40:TYR:CE1	2.52	0.44
1:D:176:ASN:HB2	6:D:568:HOH:O	2.17	0.44
1:C:271:LYS:N	1:C:272:PRO:CD	2.80	0.44
1:D:206:ILE:CD1	1:D:242:LEU:CG	2.89	0.44
1:D:179:LEU:HD11	1:D:215:LYS:NZ	2.32	0.44
1:A:257:TYR:HA	1:A:278:TRP:CZ2	2.52	0.44
1:C:194:LYS:HE2	1:C:314:SER:O	2.17	0.44
1:D:269:GLU:HG2	1:D:270:TYR:CD1	2.53	0.44
1:D:14:LYS:HA	1:D:310:LYS:HD2	2.00	0.43
1:B:173:ALA:HB2	1:B:199:HIS:O	2.18	0.43
1:B:1[B]:MET:H2	1:B:10:SER:CB	2.31	0.43
1:B:286:ASP:C	1:B:286:ASP:OD1	2.61	0.43
1:D:160:ASN:OD1	5:D:405:GOL:C2	2.64	0.43
1:A:303:THR:HA	1:A:307:GLU:HB2	2.01	0.43
1:C:33:ARG:HA	1:C:40:TYR:CE1	2.53	0.43
1:D:66:ASP:OD1	1:D:66:ASP:C	2.60	0.43
1:D:95:GLY:HA2	1:D:118:PHE:CE1	2.52	0.43
1:B:1[A]:MET:O	1:B:2[A]:ARG:CB	2.67	0.43
1:A:104[B]:PHE:CE2	1:C:262:ASP:OD1	2.57	0.43
6:A:539:HOH:O	1:C:38:HIS:HB3	2.19	0.43
4:A:403:EDO:C1	6:A:530:HOH:O	2.65	0.43
1:C:8:LYS:NZ	1:C:87:GLY:O	2.51	0.43
1:D:261:ILE:CD1	1:D:263:MET:HE2	2.47	0.43
1:C:105:TYR:O	1:C:109:ARG:NH1	2.47	0.43
1:A:149:VAL:O	1:A:153:ILE:HG13	2.18	0.42
1:B:71:GLY:O	1:D:104[B]:PHE:HE2	2.03	0.42
1:B:301:ILE:N	1:B:301:ILE:HD12	2.34	0.42
1:D:16[A]:ILE:CD1	1:D:17:GLY:O	2.67	0.42
1:D:29:SER:HB3	6:D:519:HOH:O	2.18	0.42
1:D:142:GLU:N	1:D:143:PRO:CD	2.82	0.42
1:D:206:ILE:HD11	1:D:242:LEU:HD23	1.94	0.42
1:B:177:THR:O	1:B:181:GLN:HG3	2.19	0.42
1:C:233:ASP:OD1	1:C:234:LYS:N	2.53	0.42
1:D:288:ILE:HB	1:D:289:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2[B]:ARG:HH22	1:B:13:SER:H	1.68	0.42
1:B:258:CYS:SG	1:B:261:ILE:HD12	2.59	0.42
1:D:150:GLU:O	1:D:154:ARG:HG3	2.19	0.42
1:C:234:LYS:HD3	1:C:234:LYS:HA	1.84	0.42
1:A:3:ILE:HD11	1:A:313:PHE:O	2.20	0.42
1:A:11:ILE:CD1	1:A:16:ILE:HD13	2.49	0.42
1:D:255:HIS:NE2	1:D:283:ILE:HG23	2.34	0.42
1:B:308:ASN:HB2	1:B:309:PRO:HD3	2.00	0.42
1:C:1:MET:O	1:C:2[B]:ARG:HB2	2.19	0.42
1:C:230:LEU:HA	1:C:231:PRO:HD3	1.95	0.42
1:D:179:LEU:HD11	1:D:215:LYS:HZ2	1.85	0.42
1:D:196:LEU:HD13	1:D:252:MET:CE	2.50	0.41
1:B:163:THR:O	1:B:164:LYS:HB2	2.20	0.41
1:D:2[B]:ARG:CD	1:D:2[B]:ARG:C	2.93	0.41
1:D:154:ARG:NH2	1:D:188:GLU:OE2	2.44	0.41
1:C:223:ARG:HG2	1:C:226:LEU:HD12	2.01	0.41
1:C:229:PHE:O	1:C:230:LEU:HB2	2.21	0.41
1:A:23:GLU:O	1:A:66:ASP:HA	2.20	0.41
1:D:8:LYS:NZ	1:D:87:GLY:O	2.47	0.41
1:B:33:ARG:HG3	1:B:40:TYR:CD1	2.55	0.41
1:D:146:THR:OG1	1:D:149:VAL:HG23	2.21	0.41
1:A:264:GLY:HA3	1:C:107:LEU:O	2.21	0.40
1:A:288:ILE:HB	1:A:289:PRO:HD3	2.02	0.40
1:D:16[A]:ILE:C	1:D:16[A]:ILE:CD1	2.93	0.40
1:C:23:GLU:O	1:C:66:ASP:HA	2.21	0.40
1:B:95:GLY:HA2	1:B:118:PHE:CE1	2.56	0.40
1:D:21:ILE:HG13	1:D:21:ILE:O	2.22	0.40
1:D:191:ASP:OD1	1:D:191:ASP:C	2.64	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	314/314 (100%)	300 (96%)	14 (4%)	0	100	100
1	B	313/314 (100%)	297 (95%)	12 (4%)	4 (1%)	9	8
1	C	314/314 (100%)	299 (95%)	12 (4%)	3 (1%)	12	11
1	D	315/314 (100%)	298 (95%)	15 (5%)	2 (1%)	21	23
All	All	1256/1256 (100%)	1194 (95%)	53 (4%)	9 (1%)	21	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2[A]	ARG
1	C	2[B]	ARG
1	B	266	ALA
1	B	267	LYS
1	D	266	ALA
1	D	267	LYS
1	B	2[A]	ARG
1	B	2[B]	ARG
1	C	268	PRO

5.3.2 Protein sidechains ⓘ

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	276/272 (102%)	274 (99%)	2 (1%)	76	87
1	B	275/272 (101%)	268 (98%)	7 (2%)	42	56
1	C	275/272 (101%)	268 (98%)	7 (2%)	42	56
1	D	276/272 (102%)	269 (98%)	7 (2%)	42	56
All	All	1102/1088 (101%)	1079 (98%)	23 (2%)	55	63

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	A	254	SER

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Mol	Chain	Res	Type
1	B	1[A]	MET
1	B	1[B]	MET
1	B	2[A]	ARG
1	B	2[B]	ARG
1	B	200	LEU
1	B	254	SER
1	B	260	THR
1	C	1	MET
1	C	2[A]	ARG
1	C	2[B]	ARG
1	C	12	GLU
1	C	254	SER
1	C	301[A]	ILE
1	C	301[B]	ILE
1	D	2[A]	ARG
1	D	2[B]	ARG
1	D	107	LEU
1	D	169	THR
1	D	254	SER
1	D	277[A]	ARG
1	D	277[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	58	GLN
1	A	127	GLN
1	A	131	ASN
1	A	176	ASN
1	A	182	GLN
1	A	294	ASN
1	B	127	GLN
1	B	131	ASN
1	B	176	ASN
1	B	182	GLN
1	C	51	ASN
1	C	108	ASN
1	C	127	GLN
1	C	131	ASN
1	C	182	GLN
1	C	294	ASN

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Mol	Chain	Res	Type
1	D	58	GLN
1	D	127	GLN
1	D	131	ASN
1	D	182	GLN
1	D	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	KCX	D	137	1,2,3	10,11,12	2.27	2 (20%)	6,12,14	1.80	1 (16%)
1	KCX	B	137	1,2,3	10,11,12	1.32	1 (10%)	6,12,14	0.62	0
1	KCX	A	137	1,2,3	10,11,12	2.38	2 (20%)	6,12,14	1.84	1 (16%)
1	KCX	C	137	1,2,3	10,11,12	1.83	2 (20%)	6,12,14	0.54	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
1	KCX	D	137	1,2,3	-	0/9/10/12	-
1	KCX	B	137	1,2,3	-	1/9/10/12	-
1	KCX	A	137	1,2,3	-	0/9/10/12	-
1	KCX	C	137	1,2,3	-	1/9/10/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	KCX	OQ1-CX	6.35	1.33	1.21
1	D	137	KCX	OQ1-CX	6.20	1.33	1.21
1	C	137	KCX	OQ1-CX	4.37	1.29	1.21
1	B	137	KCX	OQ1-CX	3.15	1.27	1.21
1	A	137	KCX	CE-NZ	2.31	1.51	1.46
1	C	137	KCX	CB-CA	2.17	1.56	1.53
1	D	137	KCX	CX-NZ	2.15	1.39	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	KCX	OQ1-CX-NZ	-4.40	118.24	124.92
1	D	137	KCX	OQ1-CX-NZ	-4.30	118.39	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	137	KCX	C-CA-CB-CG
1	C	137	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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
5	GOL	D	405	-	5,5,5	0.33	0	5,5,5	0.32	0
5	GOL	B	404	-	5,5,5	0.67	0	5,5,5	0.37	0
5	GOL	A	405	-	5,5,5	0.90	0	5,5,5	0.36	0
5	GOL	C	403	-	5,5,5	0.50	0	5,5,5	0.25	0
4	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.39	0
4	EDO	D	403	-	3,3,3	0.72	0	2,2,2	0.40	0
4	EDO	D	404	-	3,3,3	0.47	0	2,2,2	0.39	0
5	GOL	A	406	-	5,5,5	0.60	0	5,5,5	0.29	0
5	GOL	D	406	-	5,5,5	0.43	0	5,5,5	0.39	0
4	EDO	A	404	-	3,3,3	0.40	0	2,2,2	0.41	0
4	EDO	B	401	-	3,3,3	0.82	0	2,2,2	0.34	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
5	GOL	D	405	-	-	2/4/4/4	-
5	GOL	B	404	-	-	4/4/4/4	-
5	GOL	A	405	-	-	2/4/4/4	-
5	GOL	C	403	-	-	2/4/4/4	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	D	404	-	-	1/1/1/1	-
5	GOL	A	406	-	-	4/4/4/4	-
5	GOL	D	406	-	-	3/4/4/4	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	B	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	GOL	C1-C2-C3-O3
5	A	406	GOL	C1-C2-C3-O3
5	A	406	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	404	GOL	O1-C1-C2-C3
5	B	404	GOL	C1-C2-C3-O3
5	C	403	GOL	O1-C1-C2-O2
5	C	403	GOL	O1-C1-C2-C3
5	D	406	GOL	O1-C1-C2-C3
5	A	406	GOL	O1-C1-C2-C3
5	D	405	GOL	C1-C2-C3-O3
5	D	406	GOL	C1-C2-C3-O3
5	A	406	GOL	O1-C1-C2-O2
5	B	404	GOL	O1-C1-C2-O2
5	B	404	GOL	O2-C2-C3-O3
5	D	406	GOL	O1-C1-C2-O2
5	A	405	GOL	O2-C2-C3-O3
5	D	405	GOL	O2-C2-C3-O3
4	D	404	EDO	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	405	GOL	2	0
5	B	404	GOL	2	0
5	C	403	GOL	1	0
4	A	403	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	313/314 (99%)	-0.39	14 (4%) 38 35	16, 28, 55, 111	5 (1%)
1	B	313/314 (99%)	-0.36	10 (3%) 50 47	19, 30, 54, 114	4 (1%)
1	C	313/314 (99%)	-0.28	7 (2%) 62 59	18, 33, 59, 106	3 (0%)
1	D	313/314 (99%)	-0.19	12 (3%) 44 41	17, 33, 63, 106	4 (1%)
All	All	1252/1256 (99%)	-0.31	43 (3%) 48 45	16, 31, 59, 114	16 (1%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	266	ALA	4.2
1	C	1	MET	4.2
1	D	1	MET	4.1
1	B	266	ALA	3.8
1	A	1[A]	MET	3.7
1	A	104[A]	PHE	3.7
1	D	266	ALA	3.6
1	A	270	TYR	3.6
1	D	104[A]	PHE	3.5
1	B	1[A]	MET	3.5
1	B	2[A]	ARG	3.4
1	A	261	ILE	3.3
1	C	268	PRO	3.3
1	A	274	LEU	3.1
1	D	264	GLY	3.1
1	D	268	PRO	3.0
1	B	265	THR	2.9
1	D	263	MET	2.9
1	A	266	ALA	2.8
1	B	270	TYR	2.8
1	B	268	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	2[A]	ARG	2.7
1	C	260	THR	2.6
1	A	263	MET	2.5
1	D	270	TYR	2.5
1	B	258	CYS	2.5
1	D	274	LEU	2.4
1	A	259	CYS	2.4
1	B	260	THR	2.3
1	D	261	ILE	2.3
1	A	268	PRO	2.3
1	A	272	PRO	2.2
1	A	260	THR	2.2
1	C	270	TYR	2.2
1	C	265	THR	2.2
1	C	2[A]	ARG	2.1
1	B	263	MET	2.1
1	D	272	PRO	2.1
1	A	264	GLY	2.1
1	A	265	THR	2.1
1	D	265	THR	2.1
1	B	264	GLY	2.1
1	D	259	CYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	A	137	12/13	0.97	0.05	18,19,21,21	0
1	KCX	B	137	12/13	0.98	0.04	19,20,22,24	0
1	KCX	C	137	12/13	0.98	0.05	24,25,28,29	0
1	KCX	D	137	12/13	0.98	0.05	22,24,27,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	404	4/4	0.83	0.16	52,57,61,61	0
4	EDO	D	403	4/4	0.86	0.16	31,39,43,61	0
5	GOL	D	406	6/6	0.87	0.12	53,55,57,59	0
4	EDO	B	401	4/4	0.88	0.16	46,48,49,53	0
4	EDO	D	404	4/4	0.89	0.13	39,52,54,61	0
5	GOL	C	403	6/6	0.90	0.14	45,52,52,55	0
5	GOL	A	406	6/6	0.90	0.12	38,49,52,60	0
5	GOL	D	405	6/6	0.92	0.10	45,47,48,49	0
5	GOL	A	405	6/6	0.92	0.09	29,35,36,41	0
5	GOL	B	404	6/6	0.93	0.08	35,42,44,47	0
4	EDO	A	403	4/4	0.95	0.11	38,43,47,53	0
3	CO	D	402	1/1	0.99	0.02	24,24,24,24	0
2	FE2	B	402	1/1	0.99	0.02	21,21,21,21	0
2	FE2	D	401	1/1	0.99	0.02	23,23,23,23	0
3	CO	A	402	1/1	1.00	0.01	21,21,21,21	0
3	CO	B	403	1/1	1.00	0.02	24,24,24,24	0
3	CO	C	402	1/1	1.00	0.03	30,30,30,30	0
2	FE2	C	401	1/1	1.00	0.02	22,22,22,22	0
2	FE2	A	401	1/1	1.00	0.02	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.