



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:08 PM UTC

PDB ID : 1SFF / pdb_00001sff
Title : Structure of gamma-aminobutyrate aminotransferase complex with aminooxyacetate
Authors : Liu, W.; Peterson, P.E.; Carter, R.J.; Zhou, X.; Langston, J.A.; Fisher, A.J.; Toney, M.D.
Deposited on : 2004-02-19
Resolution : 1.90 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

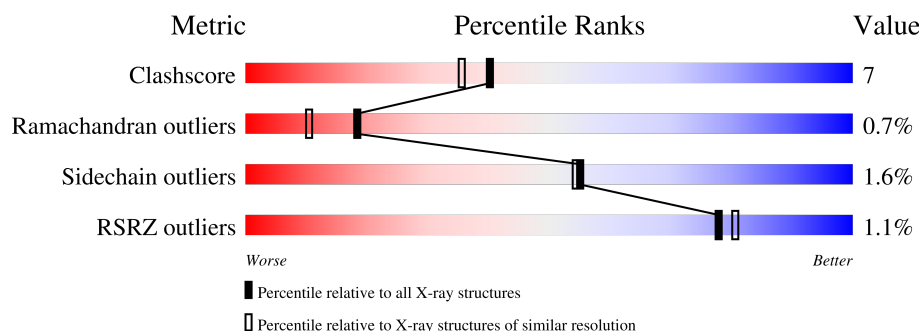
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	426	86% 13% .
1	B	426	85% 14% .
1	C	426	85% 14% .
1	D	426	84% 15% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	1401	-	-	X	-
3	EDO	B	1402	-	-	X	-
3	EDO	C	1403	-	-	X	-
3	EDO	D	1404	-	-	X	-

2 Entry composition [i](#)

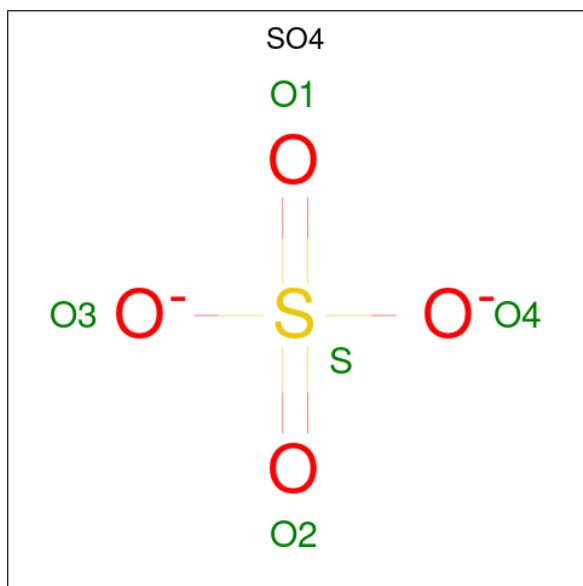
There are 5 unique types of molecules in this entry. The entry contains 14275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-aminobutyrate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	2	0
			3218	2032	563	605	18			
1	B	425	Total	C	N	O	S	0	2	0
			3218	2032	563	605	18			
1	C	425	Total	C	N	O	S	0	2	0
			3218	2032	563	605	18			
1	D	425	Total	C	N	O	S	0	2	0
			3218	2032	563	605	18			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



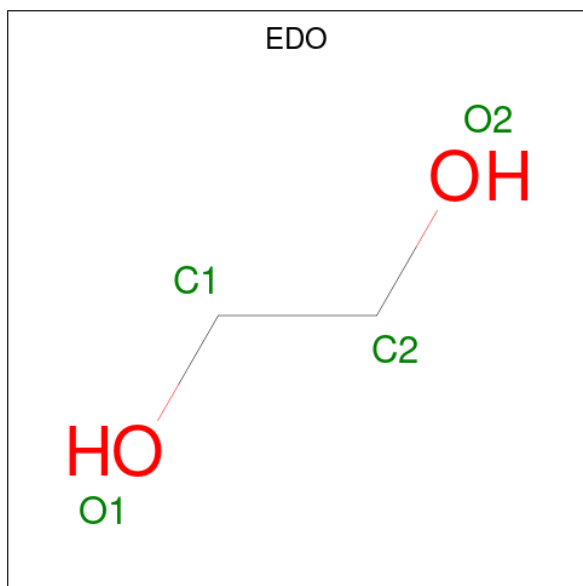
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



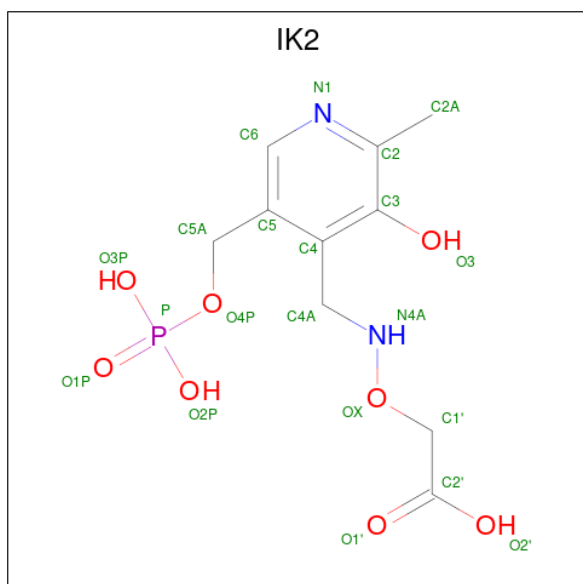
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is 4'-DEOXY-4'-ACETYLYAMINO-PYRIDOXAL-5'-PHOSPHATE (CCD ID: IK2) (formula: C₁₀H₁₅N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
4	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
4	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
4	D	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

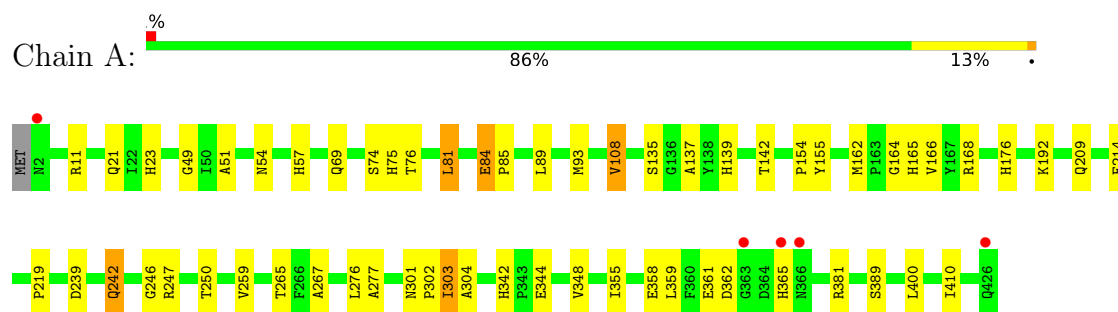
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	329	Total	O	0	0
			329	329		
5	B	316	Total	O	0	0
			316	316		
5	C	258	Total	O	0	0
			258	258		
5	D	305	Total	O	0	0
			305	305		

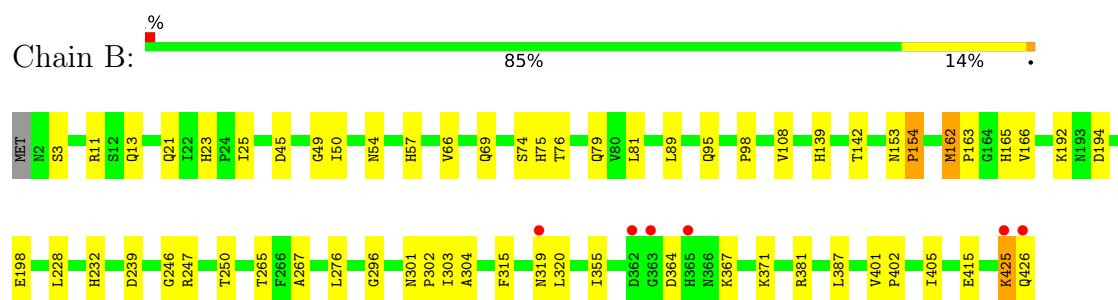
3 Residue-property plots [i](#)

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.

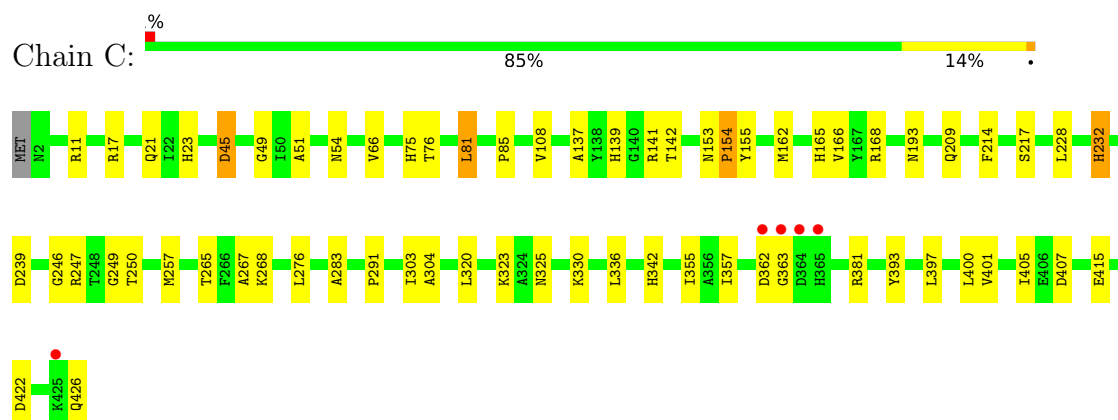
• Molecule 1: 4-aminobutyrate aminotransferase



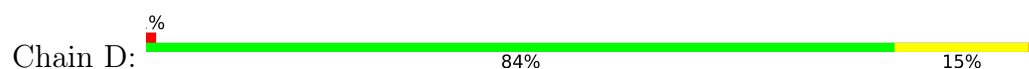
• Molecule 1: 4-aminobutyrate aminotransferase

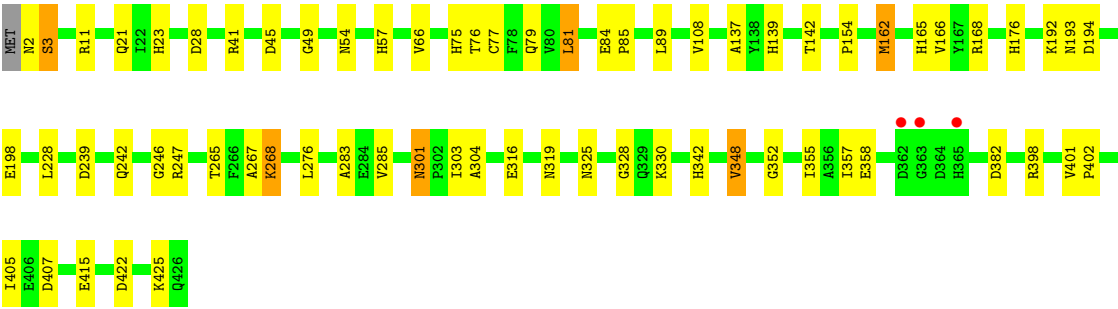


• Molecule 1: 4-aminobutyrate aminotransferase



• Molecule 1: 4-aminobutyrate aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.15Å 108.15Å 301.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 99.1 (30.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.159 , 0.186 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14275	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: SO4, EDO, IK2

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	0.85	1/3277 (0.0%)	1.04	14/4435 (0.3%)
1	B	0.86	1/3277 (0.0%)	1.03	10/4435 (0.2%)
1	C	0.77	0/3277	1.02	13/4435 (0.3%)
1	D	0.85	1/3277 (0.0%)	1.04	15/4435 (0.3%)
All	All	0.83	3/13108 (0.0%)	1.03	52/17740 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162	MET	SD-CE	6.75	1.96	1.79
1	B	162	MET	SD-CE	5.46	1.93	1.79
1	A	242	GLN	CD-OE1	5.21	1.33	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ILE	N-CA-C	-7.23	103.73	110.53
1	C	246	GLY	N-CA-C	7.03	124.71	115.36
1	D	283	ALA	N-CA-C	7.03	119.54	111.11
1	A	246	GLY	N-CA-C	6.96	124.62	115.36
1	B	246	GLY	N-CA-C	6.80	124.41	115.36
1	C	355	ILE	N-CA-C	6.80	118.84	108.71
1	D	285	VAL	N-CA-C	-6.68	104.25	110.53
1	B	166	VAL	N-CA-C	-6.31	98.54	107.75
1	D	194	ASP	N-CA-C	6.28	121.83	114.04
1	D	246	GLY	N-CA-C	6.20	123.27	115.21
1	A	155	TYR	N-CA-C	6.18	118.80	111.33
1	A	166	VAL	N-CA-C	-6.07	98.78	107.77
1	B	142	THR	N-CA-C	-5.94	101.73	110.52
1	A	342	HIS	CA-C-N	5.93	126.34	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	HIS	C-N-CA	5.93	126.34	119.47
1	D	84	GLU	N-CA-C	5.86	121.48	113.16
1	B	250	THR	N-CA-C	-5.82	100.49	109.52
1	D	355	ILE	N-CA-C	5.81	117.37	108.71
1	A	355	ILE	N-CA-C	5.78	117.65	108.87
1	D	168	ARG	N-CA-C	5.76	117.92	108.52
1	C	168	ARG	N-CA-C	5.73	117.85	108.52
1	C	141	ARG	N-CA-C	5.71	119.56	112.59
1	A	389	SER	N-CA-C	-5.69	101.76	109.95
1	C	142	THR	N-CA-C	-5.67	102.36	110.59
1	B	425	LYS	N-CA-C	-5.67	103.05	110.53
1	B	232	HIS	N-CA-C	5.62	120.14	112.88
1	A	168	ARG	N-CA-C	5.55	117.57	108.52
1	C	250	THR	N-CA-C	-5.49	101.18	109.85
1	C	166	VAL	N-CA-C	-5.46	99.69	107.77
1	A	250	THR	N-CA-C	-5.45	101.23	109.85
1	D	301	ASN	CA-C-N	5.43	124.89	119.24
1	D	301	ASN	C-N-CA	5.43	124.89	119.24
1	C	232	HIS	N-CA-C	5.41	119.57	112.92
1	C	283	ALA	N-CA-C	5.41	117.60	111.11
1	A	348	VAL	N-CA-C	-5.40	99.78	107.77
1	D	342	HIS	CA-C-N	5.32	125.64	119.47
1	D	342	HIS	C-N-CA	5.32	125.64	119.47
1	C	155	TYR	N-CA-C	5.31	117.76	111.33
1	B	98	PRO	N-CA-C	5.28	119.38	111.14
1	C	342	HIS	CA-C-N	5.28	124.94	119.56
1	C	342	HIS	C-N-CA	5.28	124.94	119.56
1	D	193	ASN	N-CA-C	5.25	119.68	113.12
1	A	84	GLU	N-CA-C	5.21	120.55	113.16
1	A	142	THR	N-CA-C	-5.21	103.04	110.59
1	B	194	ASP	N-CA-C	5.21	121.89	110.80
1	D	166	VAL	N-CA-C	-5.17	100.20	107.75
1	D	142	THR	N-CA-C	-5.10	103.19	110.59
1	B	3	SER	N-CA-C	-5.09	101.46	109.50
1	A	365	HIS	N-CA-C	5.06	118.92	112.34
1	B	355	ILE	N-CA-C	5.04	116.22	108.71
1	D	348	VAL	N-CA-C	-5.04	100.31	107.77
1	C	45	ASP	N-CA-C	5.01	116.82	107.99

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	3218	0	3229	43	0
1	B	3218	0	3229	47	0
1	C	3218	0	3229	39	0
1	D	3218	0	3229	49	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	16	0	24	6	0
3	B	12	0	18	4	0
3	C	12	0	18	8	0
3	D	16	0	24	8	0
4	A	21	0	11	0	0
4	B	21	0	11	0	0
4	C	21	0	11	0	0
4	D	21	0	11	1	0
5	A	329	0	0	7	0
5	B	316	0	0	12	0
5	C	258	0	0	7	0
5	D	305	0	0	14	0
All	All	14275	0	13044	172	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 7.

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:D:2:ASN:HD22	1:D:3:SER:H	1.15	0.94
1:C:23:HIS:HD2	1:C:381:ARG:HE	1.14	0.91
1:B:303:ILE:HG12	5:B:1672:HOH:O	1.75	0.86
1:B:198:GLU:HG3	5:B:1647:HOH:O	1.75	0.84
1:A:11:ARG:HE	1:A:21:GLN:HE21	1.27	0.83
1:D:85:PRO:HD3	3:D:1408:EDO:H22	1.60	0.82
1:D:198:GLU:HG3	5:D:1635:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HE2	1:C:393:TYR:CE2	2.14	0.80
4:D:450:IK2:N4A	5:D:1718:HOH:O	2.15	0.78
1:C:11:ARG:HE	1:C:21:GLN:HE21	1.34	0.76
3:A:1401:EDO:H12	1:B:81:LEU:HD12	1.69	0.75
1:A:76:THR:HB	3:B:1402:EDO:H11	1.71	0.73
1:D:2:ASN:HD22	1:D:3:SER:N	1.86	0.72
1:A:23:HIS:HD2	1:A:381:ARG:HE	1.35	0.71
1:B:79:GLN:HE22	1:B:296:GLY:H	1.36	0.71
1:D:11:ARG:HE	1:D:21:GLN:HE21	1.36	0.71
1:C:81:LEU:HD22	3:D:1404:EDO:H21	1.73	0.70
1:B:139:HIS:HD2	1:B:239:ASP:OD2	1.75	0.70
1:B:11:ARG:HE	1:B:21:GLN:HE21	1.38	0.69
3:A:1401:EDO:H11	1:B:76:THR:HB	1.73	0.69
1:C:76:THR:HB	3:D:1404:EDO:H22	1.75	0.68
1:B:301:ASN:ND2	5:B:1672:HOH:O	2.27	0.67
1:C:232:HIS:HD2	5:C:1637:HOH:O	1.76	0.67
1:C:23:HIS:CD2	1:C:381:ARG:HE	2.06	0.67
1:C:85:PRO:HD3	3:C:1407:EDO:H11	1.77	0.66
1:D:75:HIS:HD2	5:D:1441:HOH:O	1.77	0.66
1:C:139:HIS:HD2	1:C:239:ASP:OD2	1.78	0.66
1:D:139:HIS:HD2	1:D:239:ASP:OD2	1.79	0.65
1:A:54:ASN:ND2	1:A:247:ARG:HH11	1.93	0.65
1:D:2:ASN:ND2	1:D:3:SER:H	1.92	0.64
1:A:75:HIS:HD2	5:A:1433:HOH:O	1.80	0.64
1:C:75:HIS:HD2	5:C:1425:HOH:O	1.79	0.63
1:B:162:MET:O	1:D:165:HIS:HE1	1.80	0.63
1:B:165:HIS:HE1	1:D:162:MET:O	1.82	0.62
3:D:1408:EDO:H21	5:D:1555:HOH:O	2.00	0.62
1:B:75:HIS:HD2	5:B:1503:HOH:O	1.83	0.61
1:A:11:ARG:HE	1:A:21:GLN:NE2	1.98	0.61
3:C:1403:EDO:H22	1:D:76:THR:HB	1.82	0.61
1:A:11:ARG:NE	1:A:21:GLN:HE21	1.96	0.61
1:B:13:GLN:HG3	5:B:1636:HOH:O	2.02	0.60
1:A:139:HIS:HD2	1:A:239:ASP:OD2	1.86	0.59
3:C:1403:EDO:H21	1:D:81:LEU:HD22	1.84	0.59
1:B:426:GLN:HG2	1:B:426:GLN:O	2.02	0.59
1:B:74:SER:O	1:B:302:PRO:HD2	2.04	0.58
1:A:57:HIS:HD2	5:B:1433:HOH:O	1.86	0.58
1:D:54:ASN:ND2	1:D:247:ARG:HH11	2.01	0.58
1:A:69:GLN:HG3	1:A:303:ILE:HD12	1.85	0.57
1:C:17:ARG:HD3	5:D:1697:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HD11	1:B:381:ARG:HD3	1.86	0.57
1:B:364:ASP:OD1	1:B:367:LYS:HE3	2.04	0.57
1:B:401:VAL:HG21	1:B:405:ILE:HD12	1.87	0.57
1:A:85:PRO:HD3	3:A:1406:EDO:H11	1.86	0.57
1:A:192:LYS:CG	5:C:1586:HOH:O	2.53	0.56
1:A:165:HIS:HE1	1:C:162:MET:O	1.89	0.56
1:D:85:PRO:CD	3:D:1408:EDO:H22	2.32	0.56
1:C:54:ASN:ND2	1:C:247:ARG:HH11	2.03	0.56
1:B:11:ARG:NE	1:B:21:GLN:HE21	2.04	0.56
1:D:268:LYS:NZ	5:D:1718:HOH:O	2.39	0.55
1:D:11:ARG:NE	1:D:21:GLN:HE21	2.03	0.55
3:A:1401:EDO:C1	1:B:81:LEU:HD12	2.36	0.55
1:C:51:ALA:HB2	1:C:400:LEU:HD22	1.89	0.55
1:D:45:ASP:OD2	3:D:1404:EDO:O2	2.22	0.54
1:B:192:LYS:HG3	5:D:1597:HOH:O	2.08	0.54
1:B:228:LEU:HD23	1:B:228:LEU:C	2.34	0.53
1:C:76:THR:CB	3:D:1404:EDO:H22	2.38	0.53
1:D:192:LYS:HD2	5:D:1665:HOH:O	2.09	0.53
1:C:11:ARG:NE	1:C:21:GLN:HE21	2.04	0.53
1:B:54:ASN:ND2	1:B:247:ARG:HH11	2.07	0.53
1:D:239:ASP:HA	1:D:265:THR:OG1	2.09	0.53
1:A:242:GLN:NE2	5:A:1740:HOH:O	2.42	0.52
1:C:217[B]:SER:O	1:C:257:MET:HE1	2.10	0.52
1:A:139:HIS:HE1	5:A:1427:HOH:O	1.93	0.52
1:D:325:ASN:HD22	1:D:352:GLY:HA2	1.75	0.52
1:A:162:MET:O	1:C:165:HIS:HE1	1.93	0.51
3:C:1407:EDO:H22	1:D:28:ASP:HA	1.92	0.51
1:A:69:GLN:CG	1:A:303:ILE:HD12	2.39	0.51
1:D:41:ARG:NH2	1:D:382:ASP:O	2.43	0.51
1:D:66:VAL:HG13	1:D:303:ILE:HG23	1.91	0.51
5:A:1436:HOH:O	1:B:57:HIS:HD2	1.94	0.51
1:A:76:THR:CB	3:B:1402:EDO:H11	2.40	0.50
1:C:11:ARG:HE	1:C:21:GLN:NE2	2.05	0.50
1:B:11:ARG:HE	1:B:21:GLN:NE2	2.07	0.50
1:B:192:LYS:CD	5:D:1597:HOH:O	2.60	0.50
5:C:1421:HOH:O	1:D:57:HIS:HD2	1.94	0.50
1:B:139:HIS:HE1	5:B:1421:HOH:O	1.93	0.49
1:C:139:HIS:HE1	5:C:1415:HOH:O	1.95	0.49
1:C:239:ASP:HA	1:C:265:THR:OG1	2.12	0.49
1:D:401:VAL:HG21	1:D:405:ILE:HD12	1.95	0.49
1:D:41:ARG:HH22	1:D:382:ASP:C	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:O	1:B:426:GLN:CD	2.56	0.49
1:A:137:ALA:HB1	1:A:139:HIS:CE1	2.48	0.48
1:C:401:VAL:HG21	1:C:405:ILE:HD12	1.94	0.48
1:D:330:LYS:NZ	1:D:407:ASP:OD1	2.47	0.48
1:B:239:ASP:HA	1:B:265:THR:OG1	2.13	0.48
1:A:276:LEU:HB2	1:A:304:ALA:HB1	1.96	0.48
1:B:66:VAL:HG13	1:B:303:ILE:CG2	2.44	0.48
1:B:79:GLN:NE2	1:B:296:GLY:H	2.07	0.48
1:B:276:LEU:HB2	1:B:304:ALA:HB1	1.94	0.48
1:A:84:GLU:HG3	5:B:1470:HOH:O	2.13	0.48
1:D:139:HIS:HE1	5:D:1432:HOH:O	1.96	0.48
1:B:371:LYS:HD3	5:B:1697:HOH:O	2.14	0.47
1:A:239:ASP:HA	1:A:265:THR:OG1	2.13	0.47
1:B:319:ASN:ND2	5:B:1628:HOH:O	2.30	0.47
1:C:320:LEU:HD23	1:C:323:LYS:HD2	1.95	0.47
1:D:11:ARG:HE	1:D:21:GLN:NE2	2.10	0.47
1:D:176:HIS:HE1	1:D:358:GLU:OE1	1.98	0.47
1:D:268:LYS:HE3	5:D:1718:HOH:O	2.15	0.47
1:A:23:HIS:CD2	1:A:381:ARG:HE	2.24	0.47
1:D:11:ARG:HH21	1:D:21:GLN:NE2	2.12	0.47
1:A:11:ARG:HH21	1:A:21:GLN:NE2	2.13	0.46
1:B:45:ASP:OD2	1:B:57:HIS:HE1	1.98	0.46
1:C:330:LYS:NZ	1:C:407:ASP:OD1	2.48	0.46
1:A:192:LYS:HG2	5:C:1586:HOH:O	2.15	0.46
1:B:153:ASN:HD22	1:B:154:PRO:HA	1.80	0.46
3:C:1403:EDO:H22	1:D:76:THR:CB	2.43	0.46
1:C:49:GLY:O	1:D:75:HIS:HE1	1.98	0.46
1:D:328:GLY:HA3	1:D:352:GLY:O	2.16	0.46
1:B:23:HIS:HE1	1:B:387:LEU:O	1.99	0.46
1:C:217[A]:SER:O	1:C:257:MET:HE1	2.14	0.45
1:B:192:LYS:CG	5:D:1597:HOH:O	2.63	0.45
1:B:315:PHE:CD2	1:B:320:LEU:HB2	2.52	0.45
1:A:49:GLY:O	1:B:75:HIS:HE1	2.00	0.44
1:B:89:LEU:CD2	1:B:276:LEU:HD21	2.47	0.44
1:D:422:ASP:O	1:D:425:LYS:HG2	2.18	0.44
1:D:23:HIS:HD2	3:D:1412:EDO:O2	1.99	0.44
1:D:319:ASN:ND2	5:D:1575:HOH:O	2.50	0.44
3:C:1403:EDO:H21	1:D:81:LEU:CD2	2.47	0.44
1:B:66:VAL:HG13	1:B:303:ILE:HG23	1.99	0.44
1:A:74:SER:O	1:A:302:PRO:HD2	2.18	0.44
1:B:426:GLN:O	1:B:426:GLN:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ASP:OD2	3:C:1403:EDO:O2	2.34	0.44
1:A:108:VAL:HG23	1:A:277:ALA:HB3	1.99	0.43
3:A:1401:EDO:H11	1:B:76:THR:CB	2.43	0.43
1:B:95:GLN:NE2	5:B:1713:HOH:O	2.35	0.43
1:C:137:ALA:HB1	1:C:139:HIS:CE1	2.53	0.43
1:C:209:GLN:O	1:C:214:PHE:HA	2.18	0.43
1:C:249:GLY:HA3	1:C:325:ASN:HD21	1.83	0.43
1:A:81:LEU:HD22	3:B:1402:EDO:H12	1.99	0.43
1:C:75:HIS:HE1	1:D:49:GLY:O	2.00	0.43
1:D:45:ASP:OD2	1:D:57:HIS:HE1	2.02	0.43
1:A:164:GLY:HA2	5:A:1568:HOH:O	2.18	0.43
1:B:69:GLN:HG3	1:B:303:ILE:HD13	2.00	0.43
1:C:153:ASN:HA	1:C:154:PRO:HA	1.83	0.43
1:C:228:LEU:C	1:C:228:LEU:HD23	2.43	0.43
1:A:81:LEU:HD22	3:B:1402:EDO:H22	2.00	0.43
1:A:89:LEU:O	1:A:93:MET:HG2	2.18	0.42
1:A:176:HIS:HE1	1:A:358:GLU:OE1	2.02	0.42
1:B:153:ASN:ND2	5:B:1614:HOH:O	2.49	0.42
1:D:268:LYS:CE	5:D:1718:HOH:O	2.66	0.42
1:A:301:ASN:HD22	1:A:304:ALA:H	1.66	0.42
1:C:357:ILE:HD11	1:C:397:LEU:HD12	2.02	0.42
1:D:301:ASN:HD22	1:D:304:ALA:H	1.66	0.42
1:A:89:LEU:CD2	1:A:276:LEU:HD21	2.49	0.42
1:D:137:ALA:HB1	1:D:139:HIS:CE1	2.54	0.42
1:A:192:LYS:HG3	5:C:1586:HOH:O	2.17	0.42
1:D:348:VAL:HG22	1:D:357:ILE:HG22	2.02	0.42
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.84	0.41
1:A:75:HIS:HE1	1:B:49:GLY:O	2.03	0.41
3:A:1406:EDO:H12	5:A:1518:HOH:O	2.20	0.41
1:C:66:VAL:HG13	1:C:303:ILE:HG23	2.02	0.41
1:D:242:GLN:HE22	1:D:398:ARG:HH11	1.68	0.41
1:D:276:LEU:HB2	1:D:304:ALA:HB1	2.02	0.41
1:A:51:ALA:HB2	1:A:400:LEU:HD22	2.03	0.41
1:D:228:LEU:C	1:D:228:LEU:HD23	2.45	0.41
1:A:135:SER:HA	1:C:193:ASN:OD1	2.20	0.41
5:A:1568:HOH:O	3:C:1409:EDO:H21	2.19	0.41
1:C:422:ASP:O	1:C:426:GLN:HG3	2.21	0.41
1:A:209:GLN:O	1:A:214:PHE:HA	2.21	0.40
1:A:344:GLU:O	1:A:359:LEU:HA	2.21	0.40
1:D:77:CYS:SG	1:D:79:GLN:HG2	2.61	0.40
1:A:361:GLU:O	1:A:362:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HB2	1:C:304:ALA:HB1	2.03	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	425/426 (100%)	405 (95%)	18 (4%)	2 (0%)	24	16
1	B	425/426 (100%)	407 (96%)	15 (4%)	3 (1%)	18	10
1	C	425/426 (100%)	406 (96%)	15 (4%)	4 (1%)	14	6
1	D	425/426 (100%)	406 (96%)	16 (4%)	3 (1%)	18	10
All	All	1700/1704 (100%)	1624 (96%)	64 (4%)	12 (1%)	18	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	B	267	ALA
1	C	267	ALA
1	D	267	ALA
1	D	268	LYS
1	C	268	LYS
1	A	108	VAL
1	B	108	VAL
1	D	108	VAL
1	C	108	VAL
1	C	363	GLY
1	B	50	ILE

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	331/330 (100%)	326 (98%)	5 (2%)	57	56
1	B	331/330 (100%)	327 (99%)	4 (1%)	63	63
1	C	331/330 (100%)	326 (98%)	5 (2%)	57	56
1	D	331/330 (100%)	324 (98%)	7 (2%)	47	44
All	All	1324/1320 (100%)	1303 (98%)	21 (2%)	55	54

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	154	PRO
1	A	219	PRO
1	A	259	VAL
1	A	303	ILE
1	B	154	PRO
1	B	163	PRO
1	B	402	PRO
1	B	415	GLU
1	C	81	LEU
1	C	154	PRO
1	C	291	PRO
1	C	362	ASP
1	C	415	GLU
1	D	3	SER
1	D	81	LEU
1	D	89	LEU
1	D	154	PRO
1	D	316	GLU
1	D	402	PRO
1	D	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	21	GLN
1	A	23	HIS
1	A	32	ASN
1	A	54	ASN
1	A	57	HIS
1	A	75	HIS
1	A	139	HIS
1	A	165	HIS
1	A	176	HIS
1	A	301	ASN
1	A	325	ASN
1	B	21	GLN
1	B	23	HIS
1	B	32	ASN
1	B	54	ASN
1	B	57	HIS
1	B	75	HIS
1	B	79	GLN
1	B	95	GLN
1	B	139	HIS
1	B	153	ASN
1	B	165	HIS
1	B	176	HIS
1	B	188	HIS
1	B	209	GLN
1	B	242	GLN
1	B	317	GLN
1	B	319	ASN
1	B	325	ASN
1	B	329	GLN
1	B	366	ASN
1	B	412	GLN
1	C	21	GLN
1	C	23	HIS
1	C	32	ASN
1	C	54	ASN
1	C	75	HIS
1	C	139	HIS
1	C	165	HIS
1	C	176	HIS
1	C	209	GLN
1	C	232	HIS

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Mol	Chain	Res	Type
1	C	301	ASN
1	C	317	GLN
1	C	325	ASN
1	D	2	ASN
1	D	21	GLN
1	D	23	HIS
1	D	54	ASN
1	D	57	HIS
1	D	75	HIS
1	D	139	HIS
1	D	165	HIS
1	D	176	HIS
1	D	209	GLN
1	D	242	GLN
1	D	301	ASN
1	D	317	GLN
1	D	319	ASN
1	D	325	ASN
1	D	329	GLN
1	D	412	GLN
1	D	426	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](#)

29 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
3	EDO	A	1401	-	3,3,3	0.45	0	2,2,2	0.22	0
2	SO4	D	1306	-	4,4,4	1.85	2 (50%)	6,6,6	0.83	0
3	EDO	C	1403	-	3,3,3	0.45	0	2,2,2	0.24	0
4	IK2	D	450	-	19,21,21	2.59	6 (31%)	24,29,29	1.30	5 (20%)
2	SO4	C	1303	-	4,4,4	1.83	1 (25%)	6,6,6	0.86	0
3	EDO	D	1408	-	3,3,3	0.55	0	2,2,2	0.15	0
2	SO4	B	1302	-	4,4,4	1.87	2 (50%)	6,6,6	0.87	0
3	EDO	D	1404	-	3,3,3	0.41	0	2,2,2	0.26	0
4	IK2	B	450	-	19,21,21	2.93	7 (36%)	24,29,29	1.69	6 (25%)
3	EDO	B	1405	-	3,3,3	0.51	0	2,2,2	0.36	0
4	IK2	C	450	-	19,21,21	2.69	8 (42%)	24,29,29	1.42	4 (16%)
2	SO4	C	1309	-	4,4,4	1.86	2 (50%)	6,6,6	0.81	0
3	EDO	C	1407	-	3,3,3	0.66	0	2,2,2	0.14	0
3	EDO	B	1402	-	3,3,3	0.51	0	2,2,2	0.23	0
3	EDO	D	1412	-	3,3,3	0.61	0	2,2,2	0.20	0
2	SO4	C	1311	-	4,4,4	1.85	2 (50%)	6,6,6	0.84	0
2	SO4	D	1304	-	4,4,4	1.87	1 (25%)	6,6,6	0.84	0
4	IK2	A	450	-	19,21,21	2.53	8 (42%)	24,29,29	1.66	5 (20%)
2	SO4	B	1308	-	4,4,4	1.85	1 (25%)	6,6,6	0.87	0
3	EDO	A	1410	-	3,3,3	0.58	0	2,2,2	0.11	0
3	EDO	B	1414	-	3,3,3	0.46	0	2,2,2	0.23	0
2	SO4	A	1307	-	4,4,4	1.87	2 (50%)	6,6,6	0.80	0
2	SO4	A	1301	-	4,4,4	1.85	1 (25%)	6,6,6	0.89	0
3	EDO	C	1409	-	3,3,3	0.60	0	2,2,2	0.21	0
3	EDO	A	1411	-	3,3,3	0.55	0	2,2,2	0.25	0
2	SO4	D	1310	-	4,4,4	1.87	2 (50%)	6,6,6	0.81	0
3	EDO	A	1406	-	3,3,3	0.74	0	2,2,2	0.09	0
2	SO4	B	1305	-	4,4,4	1.86	2 (50%)	6,6,6	0.80	0
3	EDO	D	1413	-	3,3,3	0.72	0	2,2,2	0.21	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
3	EDO	A	1401	-	-	1/1/1/1	-
4	IK2	B	450	-	-	2/11/13/13	0/1/1/1
4	IK2	A	450	-	-	2/11/13/13	0/1/1/1
3	EDO	B	1405	-	-	1/1/1/1	-
3	EDO	C	1403	-	-	1/1/1/1	-
3	EDO	A	1411	-	-	1/1/1/1	-
4	IK2	C	450	-	-	2/11/13/13	0/1/1/1
4	IK2	D	450	-	-	3/11/13/13	0/1/1/1
3	EDO	A	1406	-	-	1/1/1/1	-
3	EDO	A	1410	-	-	1/1/1/1	-
3	EDO	B	1414	-	-	1/1/1/1	-
3	EDO	D	1408	-	-	1/1/1/1	-
3	EDO	C	1407	-	-	1/1/1/1	-
3	EDO	B	1402	-	-	1/1/1/1	-
3	EDO	D	1412	-	-	1/1/1/1	-
3	EDO	D	1404	-	-	1/1/1/1	-
3	EDO	D	1413	-	-	1/1/1/1	-
3	EDO	C	1409	-	-	1/1/1/1	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	450	IK2	C3-C2	7.71	1.49	1.41
4	D	450	IK2	C3-C2	6.76	1.48	1.41
4	C	450	IK2	C3-C2	6.41	1.47	1.41
4	A	450	IK2	C4A-C4	-5.16	1.44	1.52
4	A	450	IK2	C5-C4	4.99	1.47	1.40
4	A	450	IK2	C3-C2	4.72	1.45	1.41
4	B	450	IK2	C5-C4	4.60	1.46	1.40
4	B	450	IK2	C3-C4	4.54	1.46	1.40
4	C	450	IK2	C5-C4	4.49	1.46	1.40
4	C	450	IK2	C4A-C4	-4.45	1.45	1.52
4	B	450	IK2	C4A-C4	-4.40	1.45	1.52
4	C	450	IK2	C6-C5	3.92	1.45	1.37
4	D	450	IK2	C6-C5	3.87	1.45	1.37
4	B	450	IK2	C6-C5	3.83	1.45	1.37
4	D	450	IK2	C5-C4	3.83	1.45	1.40
4	D	450	IK2	C4A-C4	-3.67	1.46	1.52
4	D	450	IK2	C3-C4	3.53	1.45	1.40
4	D	450	IK2	O1'-C2'	3.46	1.33	1.22
4	A	450	IK2	O1'-C2'	3.37	1.33	1.22
4	C	450	IK2	C3-C4	3.34	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1304	SO4	O1-S	3.21	1.63	1.44
4	B	450	IK2	O1'-C2'	3.16	1.32	1.22
2	B	1302	SO4	O1-S	3.11	1.63	1.44
2	A	1301	SO4	O1-S	3.11	1.63	1.44
2	D	1310	SO4	O1-S	3.10	1.63	1.44
2	C	1303	SO4	O1-S	3.10	1.63	1.44
2	B	1308	SO4	O1-S	3.08	1.63	1.44
2	C	1309	SO4	O1-S	3.08	1.63	1.44
2	B	1305	SO4	O1-S	3.08	1.63	1.44
2	A	1307	SO4	O1-S	3.07	1.63	1.44
2	D	1306	SO4	O1-S	3.05	1.62	1.44
2	C	1311	SO4	O1-S	3.00	1.62	1.44
4	C	450	IK2	O1'-C2'	3.00	1.31	1.22
4	C	450	IK2	C2-N1	2.81	1.38	1.33
4	A	450	IK2	C2-N1	2.75	1.38	1.33
4	A	450	IK2	C6-C5	2.74	1.43	1.37
4	C	450	IK2	C2A-C2	2.73	1.54	1.50
4	A	450	IK2	C3-C4	2.40	1.43	1.40
4	A	450	IK2	O3-C3	-2.36	1.31	1.36
2	C	1311	SO4	O3-S	-2.14	1.30	1.48
4	B	450	IK2	C2-N1	2.13	1.37	1.33
2	A	1307	SO4	O3-S	-2.06	1.31	1.48
2	D	1306	SO4	O3-S	-2.06	1.31	1.48
2	B	1305	SO4	O3-S	-2.04	1.31	1.48
2	B	1302	SO4	O3-S	-2.04	1.31	1.48
2	C	1309	SO4	O3-S	-2.03	1.31	1.48
2	D	1310	SO4	O3-S	-2.03	1.31	1.48

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	450	IK2	C6-C5-C4	3.94	121.04	118.06
4	B	450	IK2	C6-C5-C4	3.91	121.02	118.06
4	B	450	IK2	C4A-C4-C3	3.66	124.84	119.98
4	B	450	IK2	C5A-C5-C6	-3.44	113.76	119.36
4	C	450	IK2	C6-C5-C4	3.43	120.66	118.06
4	A	450	IK2	C5A-C5-C6	-3.39	113.83	119.36
4	A	450	IK2	C4A-C4-C3	3.18	124.20	119.98
4	C	450	IK2	C5A-C5-C6	-2.87	114.69	119.36
4	A	450	IK2	C5-C6-N1	-2.77	119.33	123.83
4	D	450	IK2	C6-C5-C4	2.68	120.09	118.06
4	C	450	IK2	C4A-C4-C3	2.64	123.50	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	450	IK2	C5A-C5-C6	-2.52	115.25	119.36
4	D	450	IK2	C4A-C4-C3	2.45	123.23	119.98
4	B	450	IK2	C6-N1-C2	2.41	123.57	119.20
4	D	450	IK2	C5-C6-N1	-2.38	119.95	123.83
4	B	450	IK2	C5-C6-N1	-2.38	119.96	123.83
4	D	450	IK2	C6-N1-C2	2.30	123.36	119.20
4	A	450	IK2	C6-N1-C2	2.29	123.36	119.20
4	C	450	IK2	C5-C6-N1	-2.27	120.14	123.83
4	B	450	IK2	C3-C4-C5	-2.21	116.73	118.73

There are no chirality outliers.

All (23) torsion outliers are listed below:

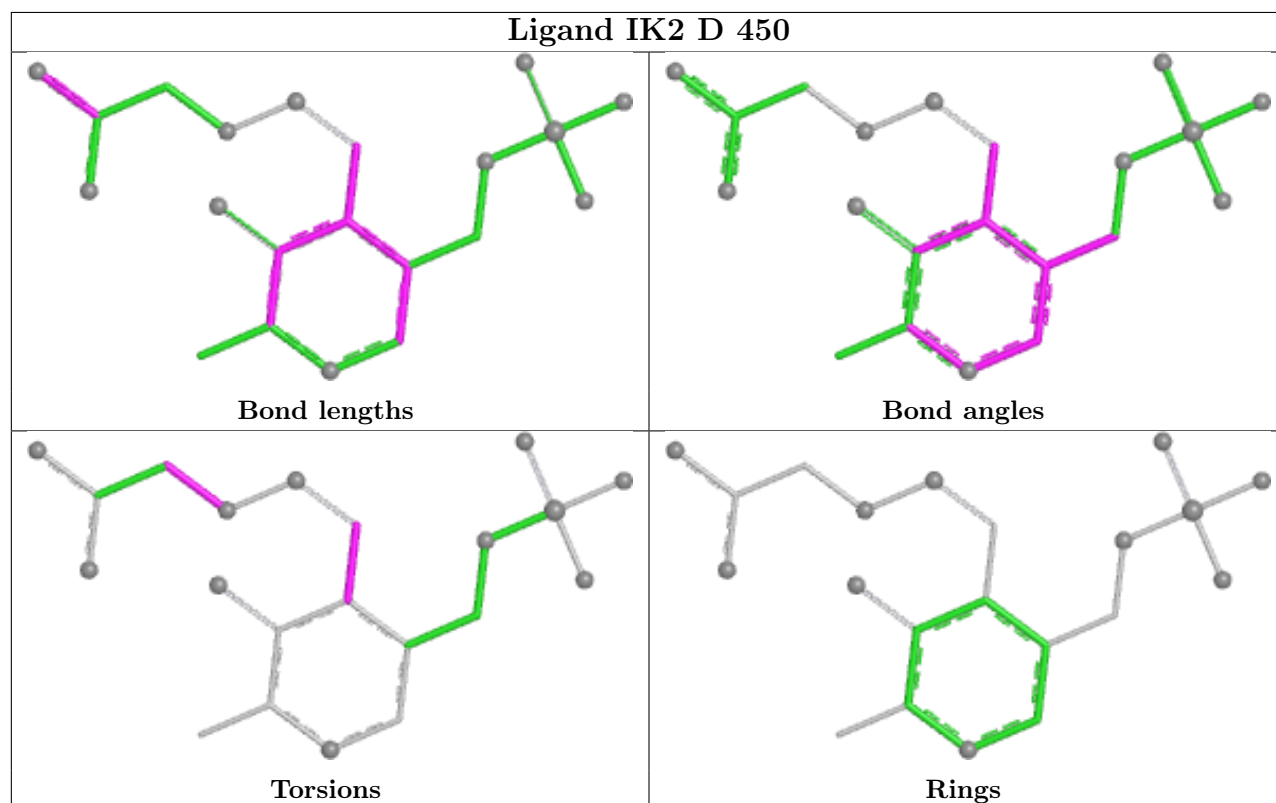
Mol	Chain	Res	Type	Atoms
4	A	450	IK2	C3-C4-C4A-N4A
4	B	450	IK2	C3-C4-C4A-N4A
4	C	450	IK2	C3-C4-C4A-N4A
4	D	450	IK2	C3-C4-C4A-N4A
4	A	450	IK2	C5-C4-C4A-N4A
4	B	450	IK2	C5-C4-C4A-N4A
4	C	450	IK2	C5-C4-C4A-N4A
4	D	450	IK2	C5-C4-C4A-N4A
3	A	1401	EDO	O1-C1-C2-O2
3	A	1406	EDO	O1-C1-C2-O2
3	A	1410	EDO	O1-C1-C2-O2
3	A	1411	EDO	O1-C1-C2-O2
3	B	1402	EDO	O1-C1-C2-O2
3	B	1405	EDO	O1-C1-C2-O2
3	B	1414	EDO	O1-C1-C2-O2
3	C	1403	EDO	O1-C1-C2-O2
3	C	1407	EDO	O1-C1-C2-O2
3	C	1409	EDO	O1-C1-C2-O2
3	D	1404	EDO	O1-C1-C2-O2
3	D	1408	EDO	O1-C1-C2-O2
3	D	1412	EDO	O1-C1-C2-O2
3	D	1413	EDO	O1-C1-C2-O2
4	D	450	IK2	C2'-C1'-OX-N4A

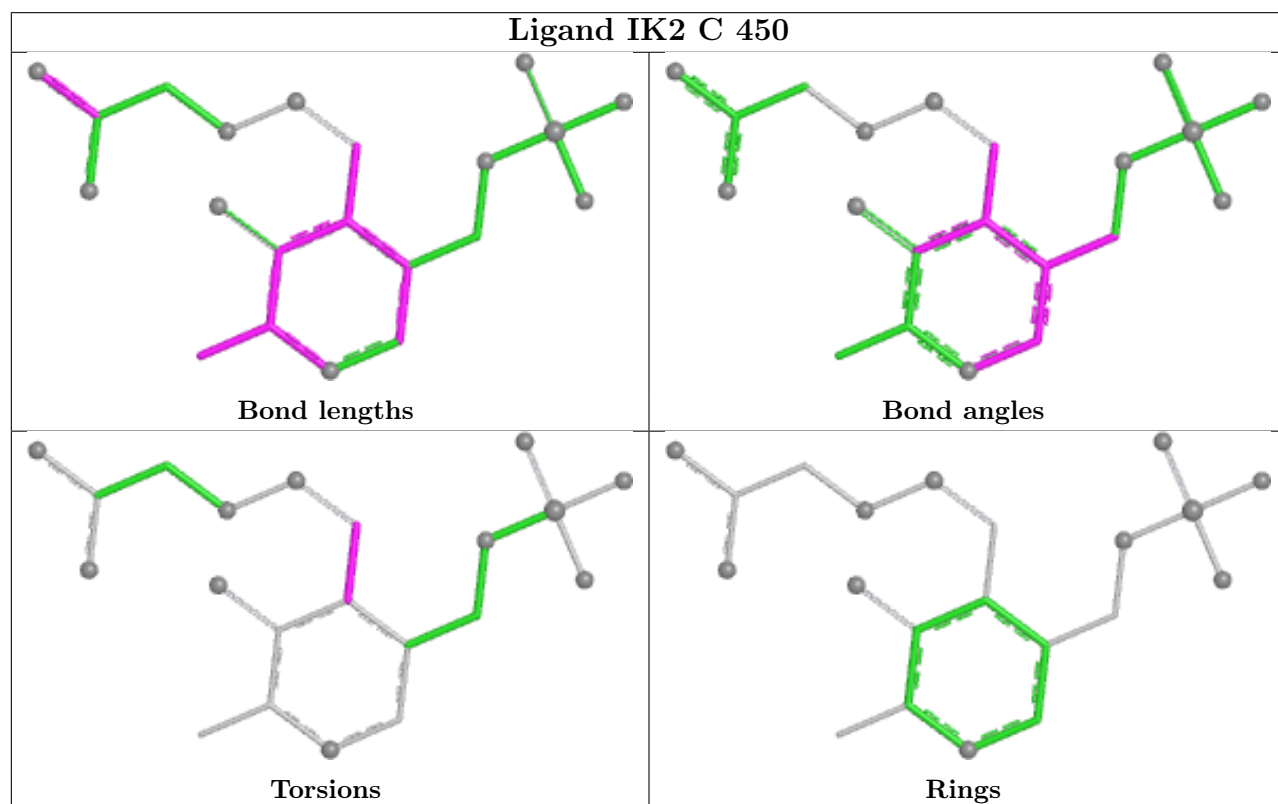
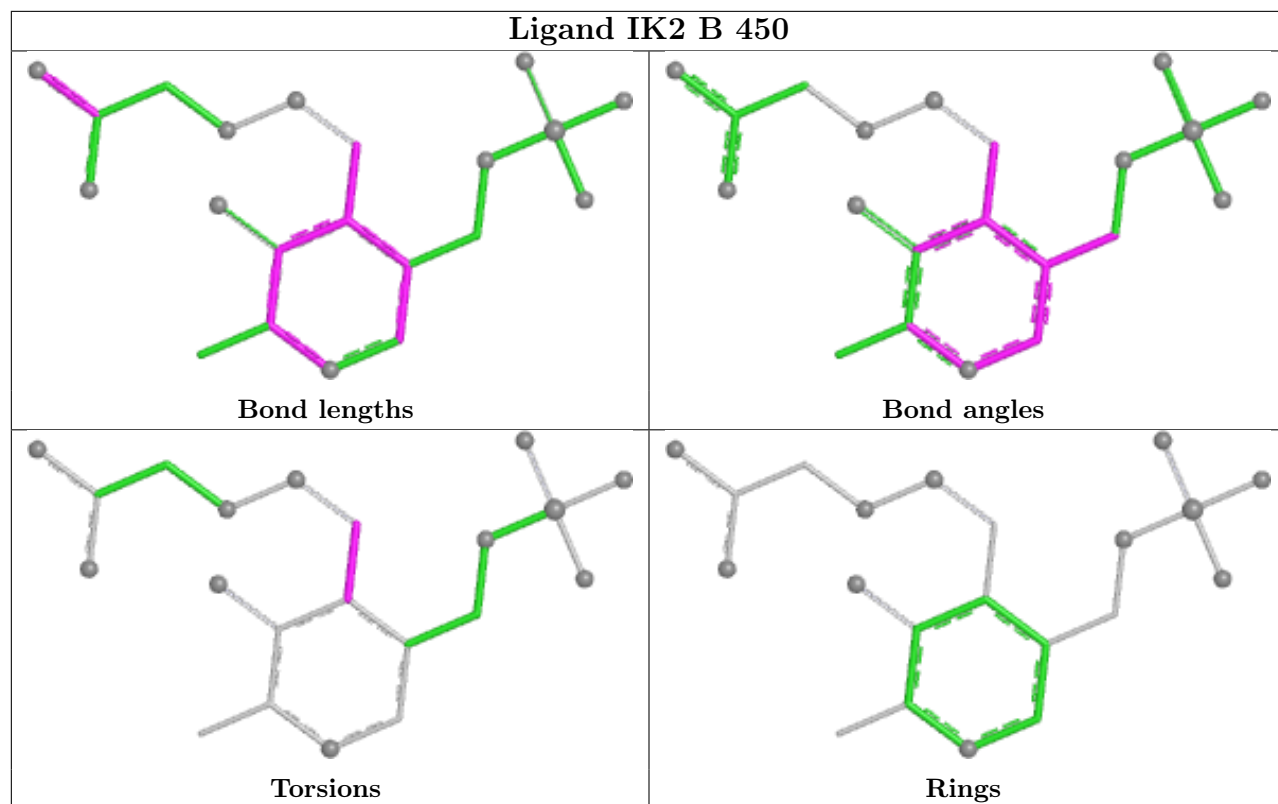
There are no ring outliers.

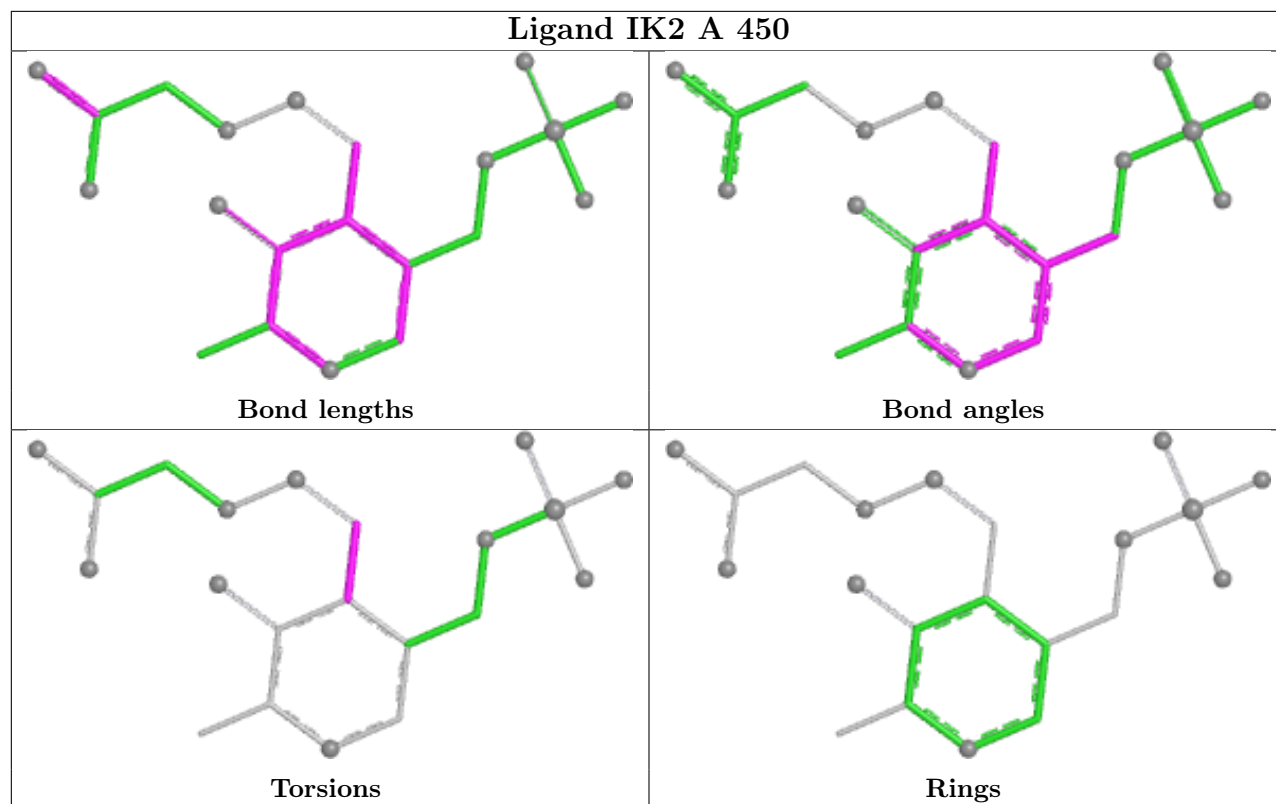
10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1401	EDO	4	0
3	C	1403	EDO	5	0
4	D	450	IK2	1	0
3	D	1408	EDO	3	0
3	D	1404	EDO	4	0
3	C	1407	EDO	2	0
3	B	1402	EDO	4	0
3	D	1412	EDO	1	0
3	C	1409	EDO	1	0
3	A	1406	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	425/426 (99%)	-0.59	5 (1%) 76 79	4, 18, 32, 61	2 (0%)
1	B	425/426 (99%)	-0.58	6 (1%) 73 76	4, 17, 34, 65	2 (0%)
1	C	425/426 (99%)	-0.42	5 (1%) 76 79	5, 21, 40, 64	2 (0%)
1	D	425/426 (99%)	-0.54	3 (0%) 84 86	4, 17, 34, 61	2 (0%)
All	All	1700/1704 (99%)	-0.53	19 (1%) 78 80	4, 18, 36, 65	8 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	GLN	3.7
1	B	363	GLY	3.5
1	D	365	HIS	3.2
1	B	365	HIS	3.1
1	B	362	ASP	3.0
1	C	365	HIS	3.0
1	D	363	GLY	2.9
1	A	365	HIS	2.9
1	A	363	GLY	2.7
1	C	363	GLY	2.7
1	A	2	ASN	2.6
1	A	366	ASN	2.6
1	B	425	LYS	2.5
1	B	319	ASN	2.5
1	C	362	ASP	2.4
1	C	425	LYS	2.3
1	D	362	ASP	2.2
1	A	426	GLN	2.1
1	C	364	ASP	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	SO4	B	1308	5/5	0.70	0.19	72,73,73,74	5
2	SO4	B	1305	5/5	0.75	0.14	78,79,79,80	0
2	SO4	C	1309	5/5	0.76	0.14	77,78,79,79	5
2	SO4	A	1307	5/5	0.77	0.16	94,94,95,95	0
2	SO4	D	1306	5/5	0.78	0.17	71,71,72,73	5
2	SO4	D	1304	5/5	0.79	0.13	64,66,68,69	0
2	SO4	D	1310	5/5	0.81	0.13	60,60,64,64	5
2	SO4	C	1303	5/5	0.82	0.11	61,61,65,66	0
3	EDO	A	1411	4/4	0.86	0.15	40,40,44,46	0
2	SO4	C	1311	5/5	0.87	0.15	53,54,54,54	5
2	SO4	B	1302	5/5	0.89	0.10	62,63,66,67	0
3	EDO	B	1414	4/4	0.89	0.13	31,32,41,41	0
3	EDO	C	1409	4/4	0.91	0.12	35,41,43,45	0
3	EDO	A	1401	4/4	0.92	0.15	21,28,30,33	0
3	EDO	D	1413	4/4	0.92	0.16	25,25,29,30	0
3	EDO	D	1412	4/4	0.93	0.11	27,33,39,40	0
3	EDO	D	1404	4/4	0.93	0.14	23,29,31,36	0
2	SO4	A	1301	5/5	0.94	0.08	47,48,52,54	0
3	EDO	C	1403	4/4	0.94	0.12	22,26,32,34	0
3	EDO	B	1405	4/4	0.94	0.11	31,34,35,35	0
3	EDO	A	1410	4/4	0.95	0.07	23,23,23,25	0
3	EDO	D	1408	4/4	0.95	0.09	21,30,32,32	0
3	EDO	C	1407	4/4	0.96	0.07	19,26,26,29	0
3	EDO	B	1402	4/4	0.96	0.08	17,24,28,29	0
3	EDO	A	1406	4/4	0.96	0.07	19,25,29,34	0
4	IK2	A	450	21/21	0.97	0.07	9,14,36,41	0
4	IK2	C	450	21/21	0.97	0.07	12,15,41,42	0

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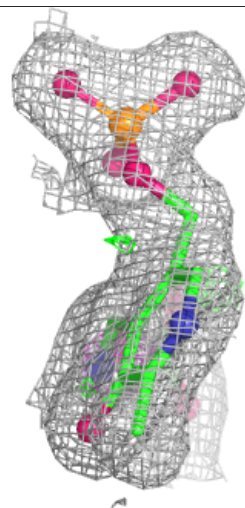
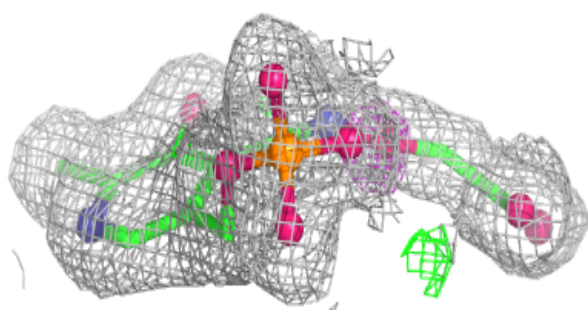
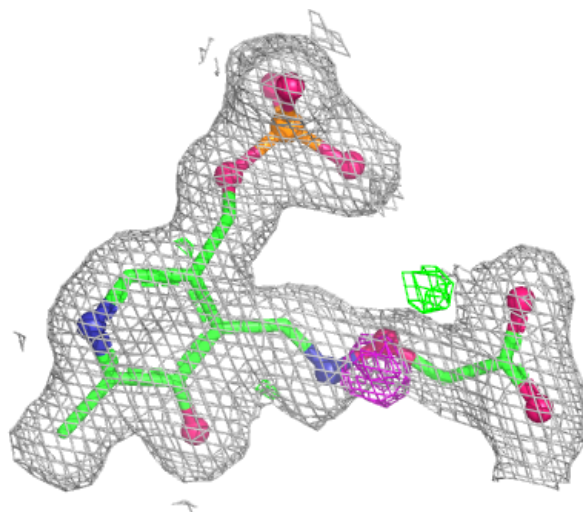
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IK2	D	450	21/21	0.97	0.07	9,14,39,47	0
4	IK2	B	450	21/21	0.98	0.06	11,15,43,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

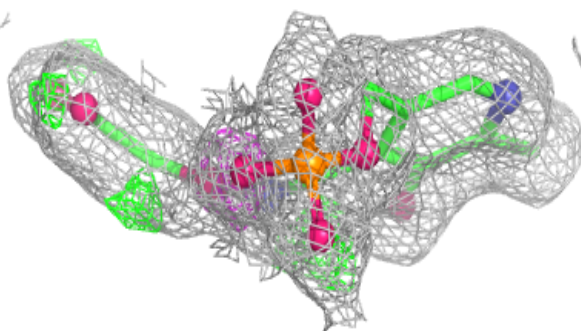
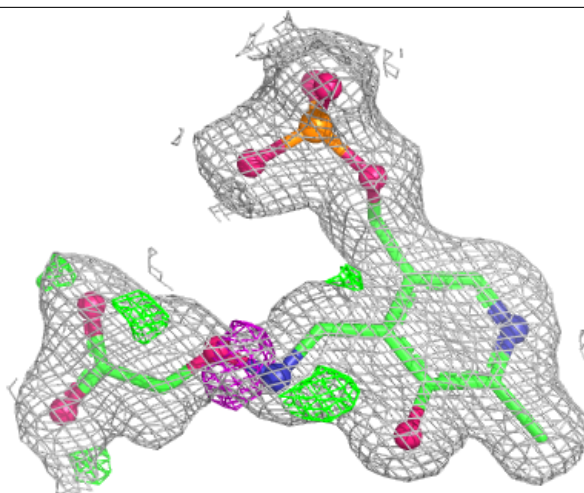
Electron density around IK2 A 450:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



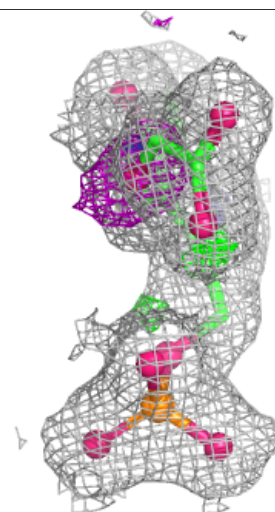
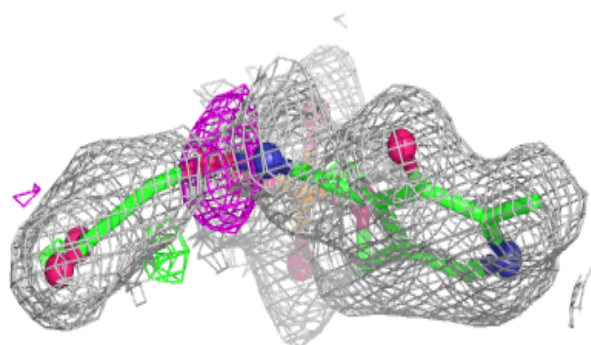
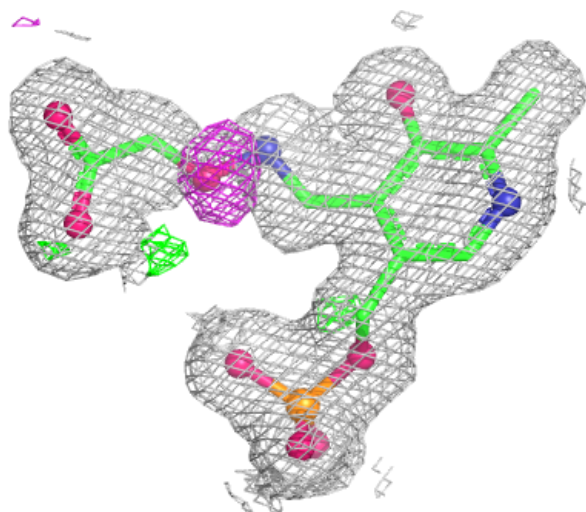
Electron density around IK2 C 450:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



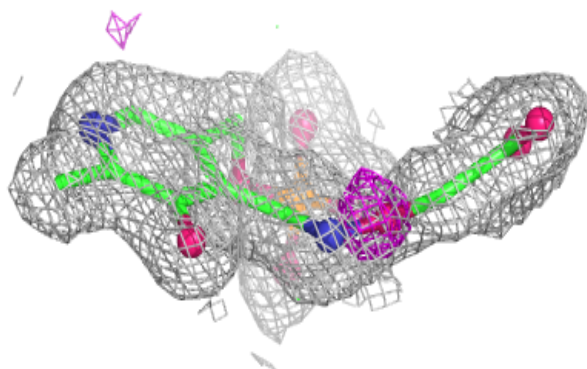
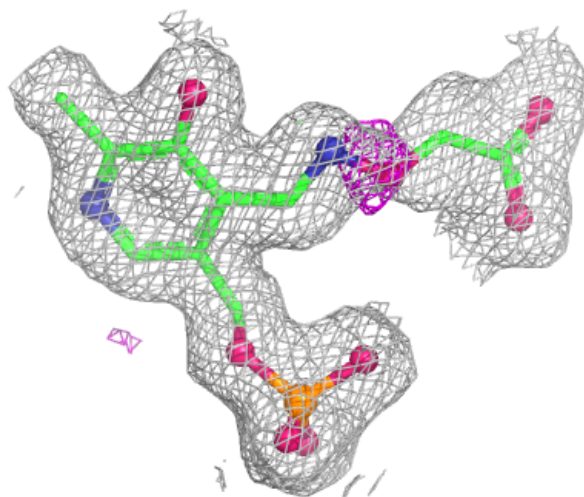
Electron density around IK2 D 450:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IK2 B 450:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.