



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:17 PM UTC

PDB ID : 3HKA / pdb_00003hka
Title : Crystal structure of uronate isomerase from *Bacillus halodurans* complexed with zinc and D-Fructuronate
Authors : Fedorov, A.A.; Fedorov, E.V.; Nguyen, T.T.; Raushel, F.M.; Almo, S.C.
Deposited on : 2009-05-22
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
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

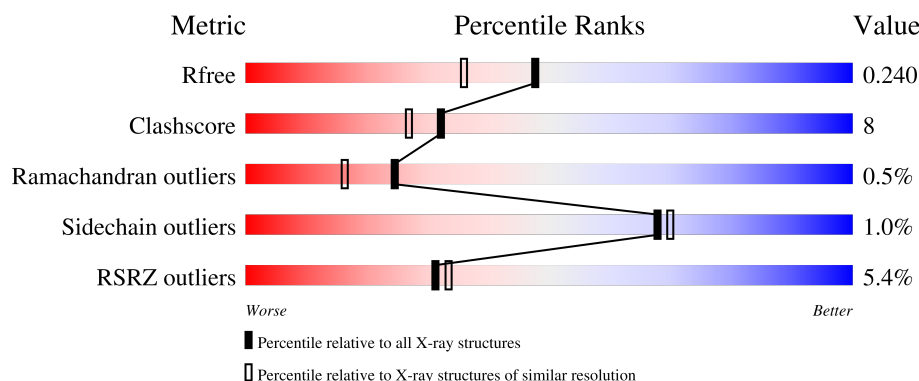
1 Overall quality at a glance

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))
R_{free}	180053	7789 (1.90-1.90)
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	427	6% 74% 20% • •
1	B	427	7% 72% 22% • •
1	C	427	2% 78% 17% • •

2 Entry composition [i](#)

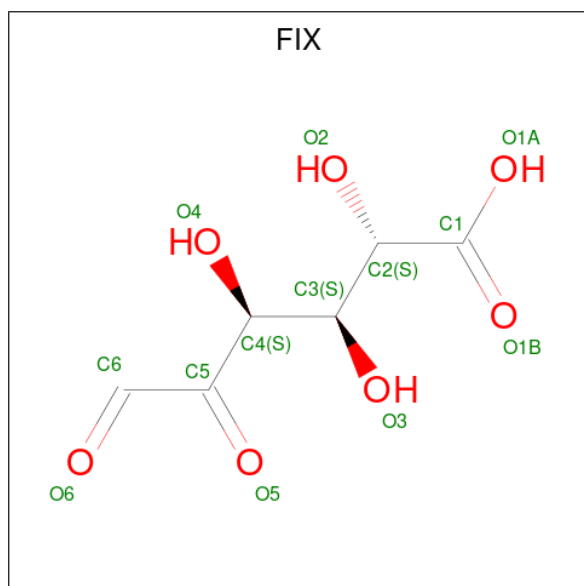
There are 6 unique types of molecules in this entry. The entry contains 10789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uronate isomerase.

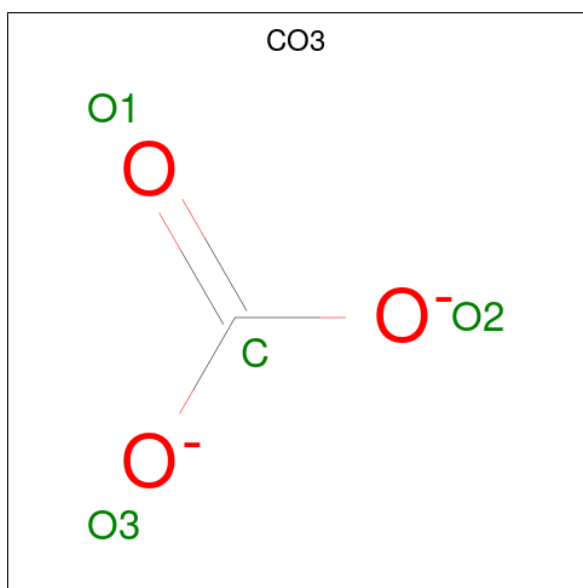
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3387	2161	583	623	20			
1	B	411	Total	C	N	O	S	0	0	0
			3387	2161	583	623	20			
1	C	411	Total	C	N	O	S	0	0	0
			3387	2161	583	623	20			

- Molecule 2 is D-fructuronic acid (CCD ID: FIX) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

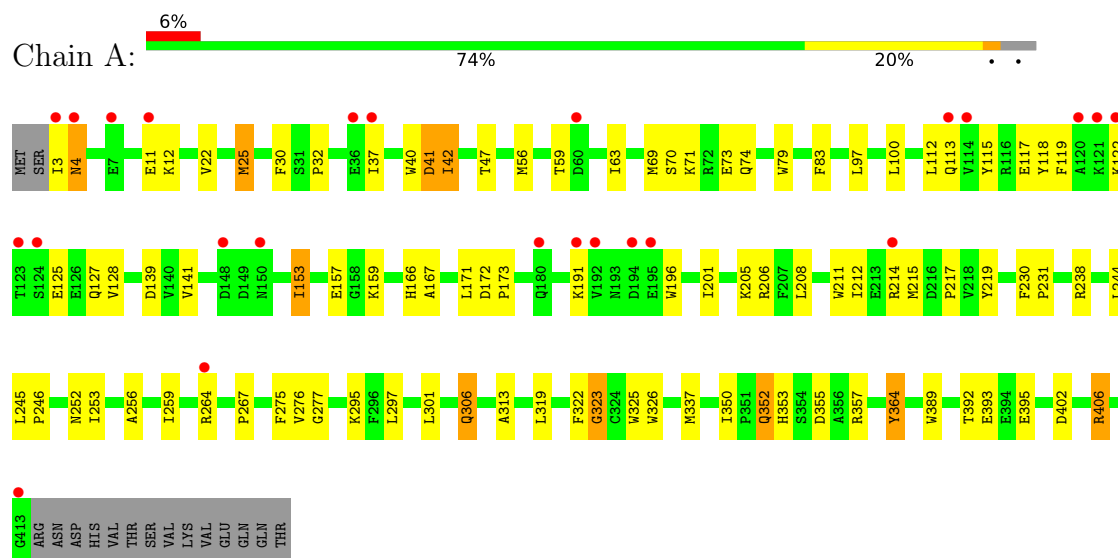
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total 171	O 171	0	0
6	B	155	Total 155	O 155	0	0
6	C	246	Total 246	O 246	0	0

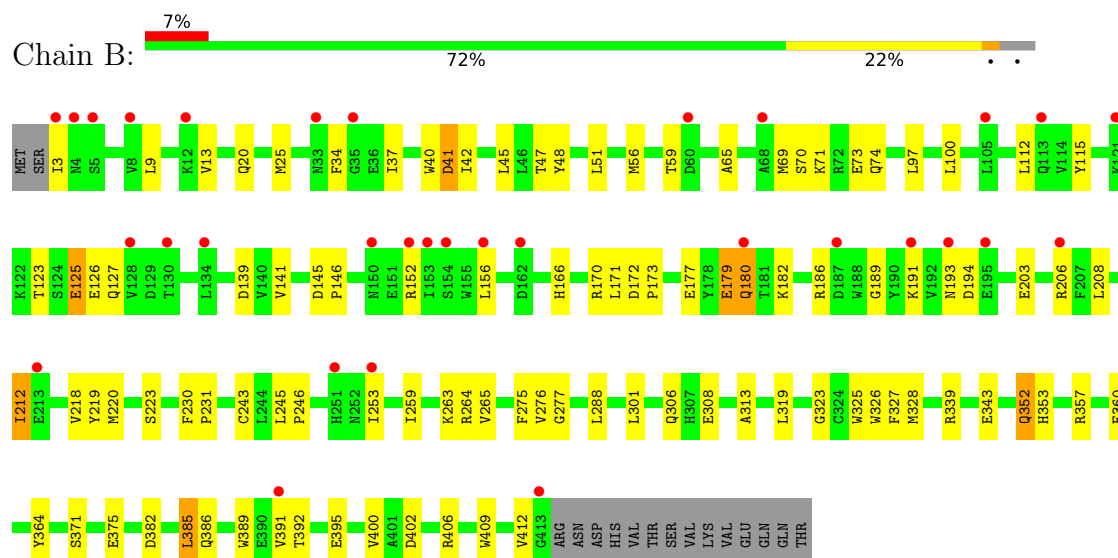
3 Residue-property plots

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.

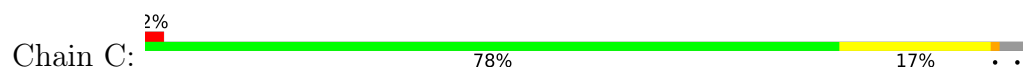
• Molecule 1: Uronate isomerase

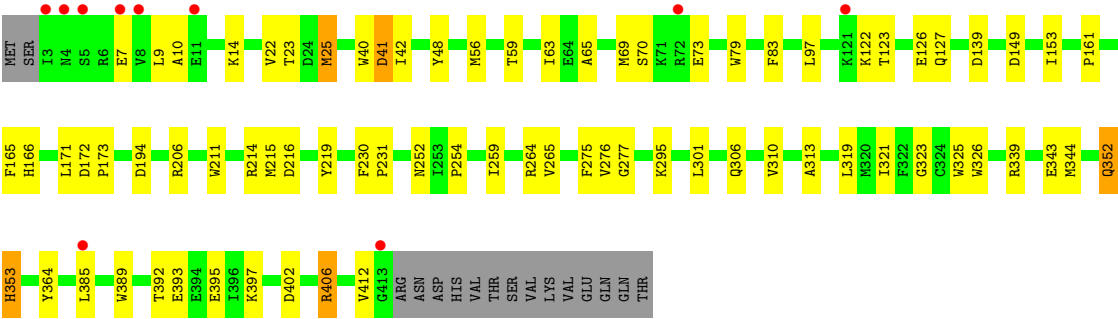


• Molecule 1: Uronate isomerase



• Molecule 1: Uronate isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.60Å 132.60Å 195.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.85 – 1.90 24.85 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (24.85-1.90) 93.9 (24.85-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.241 0.213 , 0.240	Depositor DCC
R_{free} test set	6466 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10789	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: ZN, CL, CO3, FIX

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	0.36	0/3471	0.92	13/4704 (0.3%)
1	B	0.35	0/3471	0.91	12/4704 (0.3%)
1	C	0.38	0/3471	0.95	15/4704 (0.3%)
All	All	0.36	0/10413	0.92	40/14112 (0.3%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	TRP	N-CA-C	7.92	121.84	109.96
1	C	306	GLN	N-CA-C	7.55	119.14	111.07
1	B	306	GLN	N-CA-C	7.40	118.99	111.07
1	B	325	TRP	N-CA-C	7.31	120.92	109.96
1	C	325	TRP	N-CA-C	7.23	120.80	109.96
1	C	259	ILE	N-CA-C	6.82	118.86	108.71
1	A	264	ARG	N-CA-C	6.60	120.48	111.17
1	B	259	ILE	N-CA-C	6.59	118.53	108.71
1	A	306	GLN	N-CA-C	6.53	118.06	111.07
1	C	25	MET	N-CA-C	6.49	120.91	113.19
1	C	406	ARG	N-CA-C	6.25	118.09	111.28
1	A	259	ILE	N-CA-C	6.21	117.96	108.71
1	A	25	MET	N-CA-C	6.21	120.57	113.19
1	B	352	GLN	N-CA-C	6.14	117.57	108.60
1	A	352	GLN	N-CA-C	6.10	118.13	108.79
1	C	59	THR	N-CA-C	5.98	118.94	110.50
1	C	171	LEU	N-CA-C	5.88	120.06	112.41
1	B	264	ARG	N-CA-C	5.81	119.41	111.39
1	C	22	VAL	N-CA-C	5.76	117.30	108.71
1	A	406	ARG	N-CA-C	5.68	117.47	111.28
1	C	352	GLN	N-CA-C	5.64	117.42	108.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	THR	N-CA-C	5.58	117.93	110.35
1	B	357	ARG	N-CA-C	-5.55	106.87	113.97
1	A	357	ARG	N-CA-C	-5.55	107.06	113.88
1	B	263	LYS	N-CA-C	5.52	118.23	110.23
1	A	171	LEU	N-CA-C	5.47	119.52	112.41
1	C	42	ILE	N-CA-C	5.41	116.14	110.62
1	A	122	LYS	N-CA-C	5.40	117.50	110.53
1	C	353	HIS	N-CA-C	-5.38	101.11	109.24
1	B	171	LEU	N-CA-C	5.35	119.37	112.41
1	C	23	THR	N-CA-C	-5.35	100.01	108.73
1	A	22	VAL	N-CA-C	5.33	116.66	108.71
1	B	212	ILE	N-CA-C	-5.31	105.36	110.72
1	C	264	ARG	N-CA-C	5.30	118.71	111.39
1	B	385	LEU	N-CA-C	-5.27	105.61	111.36
1	C	48	TYR	N-CA-C	-5.24	102.86	110.24
1	A	42	ILE	N-CA-C	5.18	115.90	110.62
1	A	59	THR	N-CA-C	5.18	117.39	110.35
1	B	48	TYR	N-CA-C	-5.12	102.81	110.23
1	C	194	ASP	N-CA-C	-5.06	105.76	111.28

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	3387	0	3310	59	0
1	B	3387	0	3310	65	0
1	C	3387	0	3310	41	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
2	C	13	0	6	0	0
3	A	4	0	0	0	0
3	B	8	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
5	A	1	0	0	0	0
6	A	171	0	0	4	0
6	B	155	0	0	4	0
6	C	246	0	0	4	0
All	All	10789	0	9948	162	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 8.

All (162) 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:32:PRO:HG3	1:A:128:VAL:HG21	1.58	0.86
1:B:220:MET:HE2	1:B:253:ILE:HD11	1.63	0.80
1:B:402:ASP:HA	1:B:406:ARG:HB2	1.71	0.71
1:C:402:ASP:HA	1:C:406:ARG:HB2	1.72	0.71
1:B:392:THR:OG1	1:B:395:GLU:HG3	1.92	0.70
1:A:252:ASN:HD21	1:A:295:LYS:HE3	1.57	0.69
1:C:339:ARG:O	1:C:343:GLU:HG3	1.92	0.68
1:A:402:ASP:HA	1:A:406:ARG:HB2	1.75	0.68
1:B:323:GLY:HA2	1:B:352:GLN:HA	1.77	0.66
1:A:323:GLY:HA2	1:A:352:GLN:HA	1.77	0.66
1:B:34:PHE:HB3	1:B:37:ILE:HD11	1.77	0.66
1:B:193:ASN:ND2	1:B:194:ASP:H	1.94	0.65
1:B:3:ILE:HD12	1:B:3:ILE:N	2.12	0.64
1:B:220:MET:HE2	1:B:253:ILE:CD1	2.28	0.64
1:A:70:SER:OG	1:A:73:GLU:HG3	1.98	0.64
1:A:392:THR:OG1	1:A:395:GLU:HG3	1.98	0.64
1:A:42:ILE:HD13	1:A:100:LEU:HD21	1.81	0.62
1:A:56:MET:HE2	1:A:63:ILE:HB	1.81	0.61
1:A:3:ILE:HD12	1:A:3:ILE:N	2.16	0.61
1:C:323:GLY:HA2	1:C:352:GLN:HA	1.82	0.61
1:A:112:LEU:HA	1:A:115:TYR:CD2	2.37	0.58
1:B:42:ILE:HD13	1:B:100:LEU:HD21	1.85	0.58
1:B:375:GLU:HG2	6:B:578:HOH:O	2.03	0.57
1:A:69:MET:HB3	1:A:73:GLU:HB2	1.87	0.57
1:A:301:LEU:HD11	1:A:326:TRP:HB3	1.86	0.57
1:C:313:ALA:HA	1:C:319:LEU:HD23	1.86	0.56
6:A:433:HOH:O	1:B:308:GLU:HG2	2.05	0.56
1:B:371:SER:O	1:B:375:GLU:HG3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASP:O	1:C:153:ILE:HG12	2.06	0.54
1:A:125:GLU:H	1:A:125:GLU:CD	2.16	0.54
1:C:310:VAL:HG11	1:C:344:MET:HE3	1.89	0.54
1:C:10:ALA:O	1:C:14:LYS:HG3	2.07	0.54
1:A:166:HIS:HD2	6:A:583:HOH:O	1.91	0.54
1:C:385:LEU:HD23	1:C:389:TRP:O	2.08	0.54
1:C:166:HIS:HD2	6:C:520:HOH:O	1.90	0.54
1:A:157:GLU:OE2	1:A:159:LYS:HE3	2.08	0.53
1:C:79:TRP:O	1:C:83:PHE:HB2	2.08	0.53
1:C:56:MET:HE2	1:C:63:ILE:HB	1.89	0.53
1:B:170:ARG:NH2	1:B:223:SER:HB3	2.24	0.53
1:A:276:VAL:HG22	1:A:277:GLY:N	2.25	0.52
1:A:245:LEU:HB2	1:A:246:PRO:HD3	1.91	0.52
1:B:70:SER:O	1:B:74:GLN:HG3	2.09	0.52
1:B:352:GLN:HG3	1:B:353:HIS:N	2.25	0.52
1:C:392:THR:OG1	1:C:395:GLU:HG3	2.10	0.52
1:B:182:LYS:O	1:B:186:ARG:HG3	2.10	0.51
1:B:276:VAL:HG22	1:B:277:GLY:N	2.24	0.51
1:C:219:TYR:HB3	1:C:254:PRO:HG2	1.91	0.51
1:B:328:MET:HA	1:B:328:MET:HE2	1.91	0.51
1:A:306:GLN:OE1	1:A:337:MET:HE3	2.09	0.51
1:B:152:ARG:HH11	1:B:156:LEU:HD11	1.75	0.51
1:A:40:TRP:O	1:A:41:ASP:CG	2.53	0.51
1:A:211:TRP:CE3	1:A:215:MET:HE3	2.45	0.51
1:C:127:GLN:HA	1:C:127:GLN:OE1	2.10	0.51
1:C:214:ARG:NH1	6:C:676:HOH:O	2.44	0.50
1:A:301:LEU:CD1	1:A:326:TRP:HB3	2.42	0.50
1:B:97:LEU:HD13	1:C:389:TRP:HB2	1.93	0.50
1:C:301:LEU:CD1	1:C:326:TRP:HB3	2.42	0.50
1:B:40:TRP:O	1:B:41:ASP:CG	2.55	0.50
1:C:393:GLU:HG2	1:C:397:LYS:HE3	1.94	0.50
1:C:301:LEU:HD11	1:C:326:TRP:HB3	1.93	0.49
1:A:70:SER:O	1:A:74:GLN:HG3	2.12	0.49
1:B:382:ASP:O	1:B:386:GLN:HG2	2.13	0.49
1:B:123:THR:OG1	1:B:126:GLU:HG3	2.12	0.49
1:A:113:GLN:NE2	1:A:113:GLN:HA	2.28	0.49
1:A:139:ASP:OD1	1:A:166:HIS:HE1	1.94	0.49
1:A:313:ALA:HA	1:A:319:LEU:HD23	1.94	0.49
1:B:152:ARG:NH1	1:B:156:LEU:HD11	2.28	0.49
1:A:208:LEU:O	1:A:212:ILE:HG13	2.13	0.49
1:A:25:MET:HG3	6:A:484:HOH:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:O	1:A:205:LYS:HG3	2.12	0.48
1:C:123:THR:OG1	1:C:126:GLU:HG3	2.13	0.48
1:C:265:VAL:HG21	1:C:275:PHE:HB2	1.95	0.48
1:B:9:LEU:HD22	1:B:385:LEU:HD22	1.96	0.48
1:A:352:GLN:HG3	1:A:353:HIS:N	2.27	0.48
1:B:9:LEU:O	1:B:13:VAL:HG23	2.14	0.48
1:B:313:ALA:HA	1:B:319:LEU:HD23	1.96	0.48
1:B:339:ARG:O	1:B:343:GLU:HG3	2.13	0.48
1:B:193:ASN:HD22	1:B:194:ASP:H	1.62	0.47
6:B:442:HOH:O	1:C:321:ILE:HG12	2.14	0.47
1:B:265:VAL:HG21	1:B:275:PHE:HB2	1.96	0.47
1:C:230:PHE:HA	1:C:231:PRO:C	2.39	0.47
1:A:47:THR:OG1	1:A:71:LYS:HE3	2.15	0.47
1:B:189:GLY:O	1:B:191:LYS:HD3	2.15	0.47
1:B:179:GLU:HA	1:B:179:GLU:OE1	2.15	0.47
1:C:70:SER:OG	1:C:73:GLU:HG3	2.14	0.47
1:A:113:GLN:O	1:A:117:GLU:HG3	2.14	0.47
1:A:153:ILE:HD13	1:A:153:ILE:O	2.16	0.46
1:A:172:ASP:HB2	1:A:173:PRO:HD3	1.97	0.46
1:B:139:ASP:OD1	1:B:166:HIS:HE1	1.98	0.46
1:A:97:LEU:HD13	1:B:389:TRP:HB2	1.97	0.46
1:C:40:TRP:O	1:C:41:ASP:CG	2.58	0.46
1:B:301:LEU:HD11	1:B:326:TRP:HB3	1.96	0.46
1:A:11:GLU:HG3	1:A:12:LYS:N	2.30	0.46
1:B:20:GLN:HG2	1:B:400:VAL:HG12	1.97	0.46
1:B:125:GLU:H	1:B:125:GLU:CD	2.22	0.46
1:B:245:LEU:HB2	1:B:246:PRO:HD3	1.97	0.46
1:A:219:TYR:HA	1:A:253:ILE:CG2	2.46	0.46
1:B:25:MET:HG3	6:B:455:HOH:O	2.15	0.46
1:A:30:PHE:CE2	1:A:37:ILE:HG13	2.50	0.45
1:B:409:TRP:HA	1:B:412:VAL:HG22	1.98	0.45
1:B:172:ASP:HB2	1:B:173:PRO:HD3	1.99	0.45
1:C:41:ASP:OD1	1:C:41:ASP:C	2.60	0.45
1:C:7:GLU:CD	1:C:7:GLU:H	2.25	0.45
1:B:65:ALA:O	1:B:69:MET:HG3	2.17	0.45
1:C:9:LEU:HD22	1:C:385:LEU:HD12	1.99	0.45
1:C:206:ARG:NH2	6:C:672:HOH:O	2.49	0.45
1:B:145:ASP:HA	1:B:146:PRO:HD2	1.90	0.45
1:A:115:TYR:O	1:A:118:TYR:HB3	2.17	0.44
1:B:208:LEU:O	1:B:212:ILE:HG13	2.17	0.44
1:C:139:ASP:OD1	1:C:166:HIS:HE1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASN:N	1:A:4:ASN:HD22	2.15	0.44
1:C:25:MET:HG3	6:C:465:HOH:O	2.18	0.44
1:A:12:LYS:HD2	1:A:393:GLU:CD	2.42	0.44
1:A:196:TRP:CD1	1:A:238:ARG:HD2	2.53	0.44
1:B:70:SER:OG	1:B:73:GLU:HG3	2.18	0.44
1:B:301:LEU:CD1	1:B:326:TRP:HB3	2.48	0.44
1:A:275:PHE:CG	1:A:276:VAL:N	2.85	0.44
1:A:112:LEU:HA	1:A:115:TYR:HD2	1.83	0.43
1:A:230:PHE:HA	1:A:231:PRO:C	2.43	0.43
1:B:288:LEU:HD11	1:B:319:LEU:HD22	1.99	0.43
1:C:254:PRO:HG3	1:C:412:VAL:HG12	1.99	0.43
1:A:322:PHE:HA	1:A:350:ILE:O	2.17	0.43
1:B:203:GLU:OE1	1:B:206:ARG:NH1	2.52	0.43
1:A:167:ALA:O	1:A:217:PRO:HA	2.19	0.43
1:B:391:VAL:HG23	1:B:391:VAL:O	2.18	0.43
1:C:276:VAL:HG22	1:C:277:GLY:N	2.32	0.43
1:A:25:MET:HA	1:A:141:VAL:CG2	2.48	0.43
1:C:65:ALA:O	1:C:69:MET:HG3	2.19	0.42
1:B:326:TRP:HB3	1:B:327:PHE:H	1.55	0.42
1:C:252:ASN:HD21	1:C:295:LYS:HE3	1.84	0.42
1:B:56:MET:HE3	6:B:551:HOH:O	2.19	0.42
1:C:211:TRP:CE3	1:C:215:MET:HE3	2.54	0.42
1:B:41:ASP:OD1	1:B:41:ASP:C	2.62	0.42
1:B:288:LEU:CD2	1:B:319:LEU:HB2	2.49	0.42
1:A:41:ASP:HA	1:A:119:PHE:CD1	2.55	0.42
1:B:45:LEU:HD21	1:B:360:GLU:HB2	2.02	0.42
1:C:352:GLN:HG3	1:C:353:HIS:N	2.34	0.42
1:B:127:GLN:OE1	1:B:127:GLN:HA	2.20	0.42
1:B:230:PHE:HA	1:B:231:PRO:C	2.44	0.42
1:B:243:CYS:C	1:B:246:PRO:HD2	2.45	0.41
1:C:172:ASP:HB2	1:C:173:PRO:HD3	2.02	0.41
1:B:25:MET:HE2	1:B:25:MET:HB2	1.98	0.41
1:A:41:ASP:OD1	1:A:41:ASP:C	2.62	0.41
1:A:256:ALA:HA	1:A:297:LEU:O	2.21	0.41
1:B:218:VAL:HG23	1:B:219:TYR:CD2	2.56	0.41
1:A:79:TRP:O	1:A:83:PHE:HB2	2.21	0.41
1:B:51:LEU:HD12	1:B:51:LEU:N	2.34	0.41
1:B:112:LEU:HA	1:B:115:TYR:CD2	2.56	0.41
1:C:161:PRO:HB2	1:C:165:PHE:HB2	2.02	0.41
1:B:25:MET:HA	1:B:141:VAL:CG2	2.51	0.41
1:B:177:GLU:HB3	1:B:180:GLN:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:C	1:A:244:LEU:HD13	2.45	0.41
1:A:267:PRO:HG2	6:A:532:HOH:O	2.21	0.41
1:C:215:MET:O	1:C:216:ASP:C	2.64	0.41
1:A:276:VAL:CG2	1:A:277:GLY:N	2.84	0.40
1:A:364:TYR:CD1	1:A:364:TYR:C	2.98	0.40
1:A:4:ASN:N	1:A:4:ASN:ND2	2.68	0.40
1:A:4:ASN:HD22	1:A:4:ASN:H	1.69	0.40
1:B:3:ILE:HG21	1:B:9:LEU:HB2	2.03	0.40
1:A:127:GLN:OE1	1:A:127:GLN:HA	2.21	0.40
1:B:47:THR:HG21	1:B:71:LYS:HD3	2.02	0.40
1:A:389:TRP:HB2	1:C:97:LEU:HD13	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	409/427 (96%)	397 (97%)	9 (2%)	3 (1%)	18	10
1	B	409/427 (96%)	399 (98%)	9 (2%)	1 (0%)	43	36
1	C	409/427 (96%)	398 (97%)	9 (2%)	2 (0%)	24	16
All	All	1227/1281 (96%)	1194 (97%)	27 (2%)	6 (0%)	24	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ASP
1	C	122	LYS
1	A	41	ASP
1	A	323	GLY
1	C	41	ASP
1	A	191	LYS

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	371/387 (96%)	365 (98%)	6 (2%)	55	54
1	B	371/387 (96%)	367 (99%)	4 (1%)	65	67
1	C	371/387 (96%)	370 (100%)	1 (0%)	86	88
All	All	1113/1161 (96%)	1102 (99%)	11 (1%)	68	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	153	ILE
1	A	206	ARG
1	A	214	ARG
1	A	355	ASP
1	A	364	TYR
1	B	125	GLU
1	B	179	GLU
1	B	180	GLN
1	B	364	TYR
1	C	364	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	18	ASN
1	A	20	GLN
1	A	113	GLN
1	A	133	GLN
1	A	166	HIS
1	A	183	HIS
1	A	202	GLN
1	A	252	ASN
1	A	293	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	386	GLN
1	B	15	ASN
1	B	19	ASN
1	B	20	GLN
1	B	101	GLN
1	B	136	ASN
1	B	166	HIS
1	B	193	ASN
1	B	293	ASN
1	C	15	ASN
1	C	18	ASN
1	C	20	GLN
1	C	166	HIS
1	C	202	GLN
1	C	252	ASN
1	C	293	ASN

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](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CO3	B	430	-	3,3,3	0.70	0	2,3,3	0.08	0
2	FIX	B	428	4	12,12,12	3.08	3 (25%)	12,16,16	3.36	2 (16%)
2	FIX	A	428	4	12,12,12	3.08	3 (25%)	12,16,16	3.29	2 (16%)
3	CO3	B	429	-	3,3,3	0.82	0	2,3,3	0.02	0
2	FIX	C	428	4	12,12,12	3.12	3 (25%)	12,16,16	3.21	2 (16%)
3	CO3	A	429	-	3,3,3	0.75	0	2,3,3	0.17	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	FIX	A	428	4	-	1/14/18/18	-
2	FIX	B	428	4	-	5/14/18/18	-
2	FIX	C	428	4	-	5/14/18/18	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	428	FIX	O6-C6	9.82	1.43	1.22
2	B	428	FIX	O6-C6	9.59	1.43	1.22
2	A	428	FIX	O6-C6	9.47	1.42	1.22
2	C	428	FIX	C6-C5	2.69	1.53	1.46
2	A	428	FIX	C4-C5	2.68	1.56	1.53
2	B	428	FIX	C6-C5	2.52	1.52	1.46
2	A	428	FIX	C6-C5	2.50	1.52	1.46
2	B	428	FIX	C4-C5	2.44	1.55	1.53
2	C	428	FIX	C4-C5	2.36	1.55	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	428	FIX	O6-C6-C5	-10.68	111.20	124.37
2	A	428	FIX	O6-C6-C5	-10.44	111.51	124.37
2	C	428	FIX	O6-C6-C5	-10.06	111.97	124.37
2	C	428	FIX	C4-C3-C2	2.95	116.53	112.71
2	A	428	FIX	C4-C3-C2	2.84	116.40	112.71
2	B	428	FIX	C4-C3-C2	2.79	116.33	112.71

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	428	FIX	O4-C4-C5-O5
2	B	428	FIX	O4-C4-C5-O5
2	C	428	FIX	O4-C4-C5-O5
2	B	428	FIX	O1B-C1-C2-O2
2	C	428	FIX	O1B-C1-C2-C3
2	B	428	FIX	O1A-C1-C2-C3
2	B	428	FIX	O1B-C1-C2-C3
2	C	428	FIX	O1B-C1-C2-O2
2	B	428	FIX	O1A-C1-C2-O2
2	C	428	FIX	O1A-C1-C2-C3
2	C	428	FIX	O1A-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	411/427 (96%)	0.39	24 (5%)	29 30	14, 28, 46, 62	0
1	B	411/427 (96%)	0.48	32 (7%)	19 20	15, 29, 49, 75	0
1	C	411/427 (96%)	0.02	10 (2%)	59 63	13, 22, 37, 68	0
All	All	1233/1281 (96%)	0.30	66 (5%)	31 33	13, 26, 45, 75	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ILE	6.7
1	B	3	ILE	5.7
1	C	4	ASN	4.4
1	A	122	LYS	4.0
1	B	193	ASN	3.8
1	A	37	ILE	3.5
1	A	413	GLY	3.5
1	B	8	VAL	3.5
1	C	413	GLY	3.4
1	A	123	THR	3.4
1	B	253	ILE	3.3
1	A	60	ASP	3.2
1	B	162	ASP	3.1
1	C	385	LEU	3.1
1	A	120	ALA	3.1
1	B	156	LEU	2.9
1	B	150	ASN	2.9
1	B	180	GLN	2.9
1	A	11	GLU	2.9
1	A	3	ILE	2.9
1	B	413	GLY	2.9
1	B	4	ASN	2.8
1	A	214	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	152	ARG	2.8
1	C	121	LYS	2.8
1	C	5	SER	2.8
1	A	180	GLN	2.7
1	C	8	VAL	2.7
1	B	130	THR	2.7
1	B	391	VAL	2.6
1	B	60	ASP	2.5
1	A	191	LYS	2.5
1	C	11	GLU	2.5
1	B	105	LEU	2.5
1	B	251	HIS	2.5
1	B	195	GLU	2.5
1	B	113	GLN	2.4
1	A	36	GLU	2.4
1	B	191	LYS	2.3
1	A	7	GLU	2.3
1	B	121	LYS	2.3
1	A	195	GLU	2.3
1	A	192	VAL	2.3
1	A	4	ASN	2.3
1	A	150	ASN	2.3
1	B	12	LYS	2.3
1	B	153	ILE	2.2
1	A	113	GLN	2.2
1	A	194	ASP	2.2
1	B	68	ALA	2.2
1	B	128	VAL	2.2
1	C	7	GLU	2.2
1	A	114	VAL	2.2
1	B	134	LEU	2.2
1	A	121	LYS	2.2
1	B	33	ASN	2.1
1	B	154	SER	2.1
1	B	35	GLY	2.1
1	A	264	ARG	2.1
1	B	187	ASP	2.1
1	B	206	ARG	2.1
1	C	72	ARG	2.1
1	B	5	SER	2.0
1	A	148	ASP	2.0
1	B	213	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	124	SER	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(Å ²)	Q<0.9
2	FIX	B	428	13/13	0.89	0.12	31,35,40,42	0
2	FIX	C	428	13/13	0.93	0.09	20,28,35,39	0
3	CO3	A	429	4/4	0.93	0.09	20,23,23,26	0
3	CO3	B	429	4/4	0.93	0.09	28,29,29,32	0
3	CO3	B	430	4/4	0.93	0.12	25,26,27,32	0
2	FIX	A	428	13/13	0.94	0.09	24,32,38,39	0
4	ZN	A	430	1/1	0.99	0.02	26,26,26,26	0
4	ZN	B	431	1/1	0.99	0.03	31,31,31,31	0
4	ZN	C	430	1/1	0.99	0.05	18,18,18,18	1
5	CL	A	431	1/1	0.99	0.03	14,14,14,14	0
4	ZN	C	429	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.