



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:48 AM UTC

PDB ID : 3P93 / pdb_00003p93
Title : Crystal structure of D-mannonate dehydratase from Chromohalobacter Salax-
igens complexed with MG,D-Mannonate and 2-keto-3-deoxy-D-Gluconat
e
Authors : Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2010-10-15
Resolution : 1.80 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

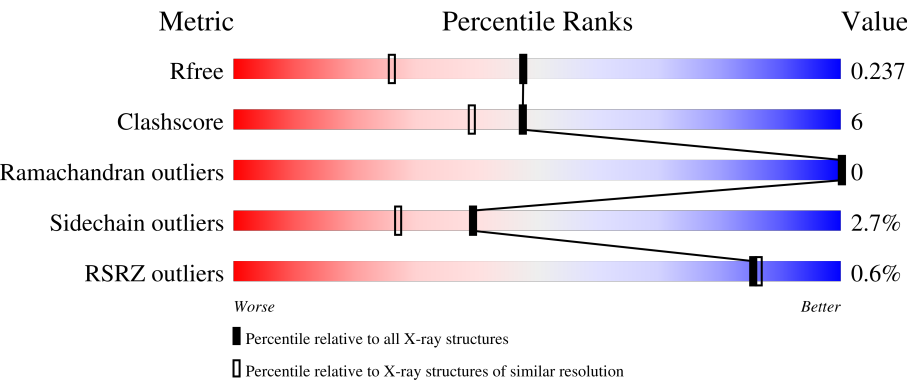
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	405	80%14%• 5%
1	B	405	% 83%12%• •
1	C	405	% 82%11%• 5%
1	D	405	% 83%11%• 5%
1	E	405	84%10%• •

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Mol	Chain	Length	Quality of chain
1	F	405	 82%11% • 5%
1	G	405	 82%12% • 5%
1	H	405	 82%11% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26363 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3043	1929	545	555	14			
1	B	388	Total	C	N	O	S	0	0	0
			3072	1946	549	563	14			
1	C	384	Total	C	N	O	S	0	0	0
			3043	1929	545	555	14			
1	D	384	Total	C	N	O	S	0	0	0
			3043	1929	545	555	14			
1	E	388	Total	C	N	O	S	0	0	0
			3072	1946	549	563	14			
1	F	383	Total	C	N	O	S	0	0	0
			3037	1926	544	553	14			
1	G	383	Total	C	N	O	S	0	0	0
			3037	1926	544	553	14			
1	H	383	Total	C	N	O	S	0	0	0
			3037	1926	544	553	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q1QT89
A	2	SER	-	expression tag	UNP Q1QT89
A	3	LEU	-	expression tag	UNP Q1QT89
B	1	MET	-	expression tag	UNP Q1QT89
B	2	SER	-	expression tag	UNP Q1QT89
B	3	LEU	-	expression tag	UNP Q1QT89
C	1	MET	-	expression tag	UNP Q1QT89
C	2	SER	-	expression tag	UNP Q1QT89
C	3	LEU	-	expression tag	UNP Q1QT89
D	1	MET	-	expression tag	UNP Q1QT89
D	2	SER	-	expression tag	UNP Q1QT89
D	3	LEU	-	expression tag	UNP Q1QT89
E	1	MET	-	expression tag	UNP Q1QT89

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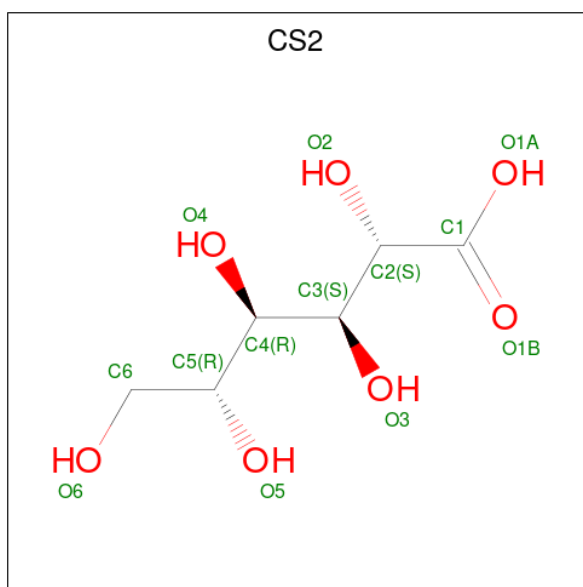
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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	SER	-	expression tag	UNP Q1QT89
E	3	LEU	-	expression tag	UNP Q1QT89
F	1	MET	-	expression tag	UNP Q1QT89
F	2	SER	-	expression tag	UNP Q1QT89
F	3	LEU	-	expression tag	UNP Q1QT89
G	1	MET	-	expression tag	UNP Q1QT89
G	2	SER	-	expression tag	UNP Q1QT89
G	3	LEU	-	expression tag	UNP Q1QT89
H	1	MET	-	expression tag	UNP Q1QT89
H	2	SER	-	expression tag	UNP Q1QT89
H	3	LEU	-	expression tag	UNP Q1QT89

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

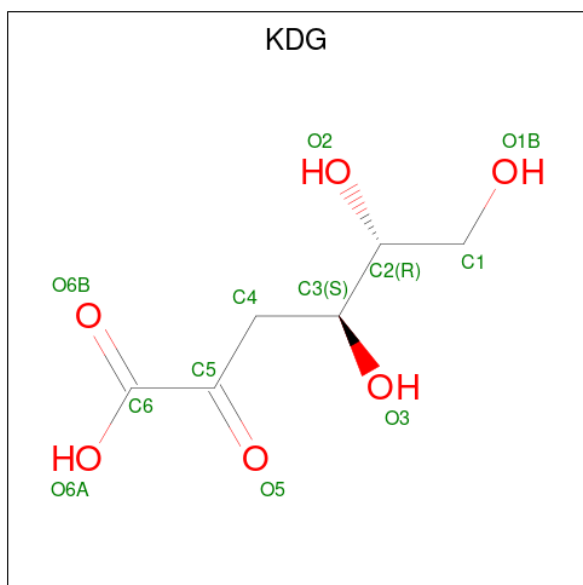
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is D-MANNONIC ACID (CCD ID: CS2) (formula: C₆H₁₂O₇).



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

- Molecule 4 is 2-KETO-3-DEOXYGLUCONATE (CCD ID: KDG) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 12 6 6	0	0
4	D	1	Total C O 12 6 6	0	0
4	G	1	Total C O 12 6 6	0	0
4	H	1	Total C O 12 6 6	0	0

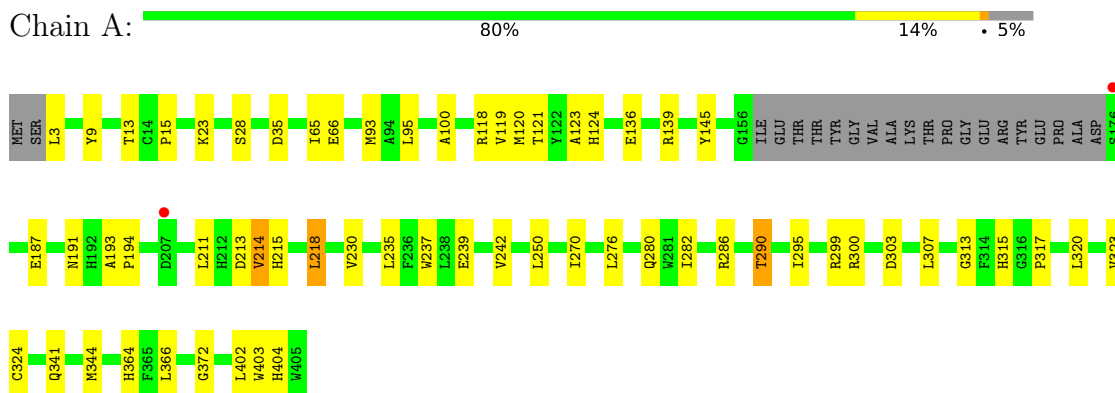
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	246	Total O 246 246	0	0
5	B	219	Total O 219 219	0	0
5	C	233	Total O 233 233	0	0
5	D	218	Total O 218 218	0	0
5	E	238	Total O 238 238	0	0
5	F	237	Total O 237 237	0	0
5	G	238	Total O 238 238	0	0
5	H	242	Total O 242 242	0	0

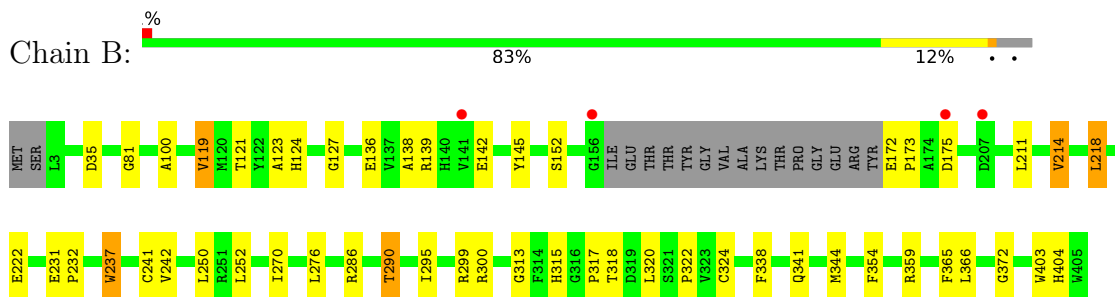
3 Residue-property plots

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.

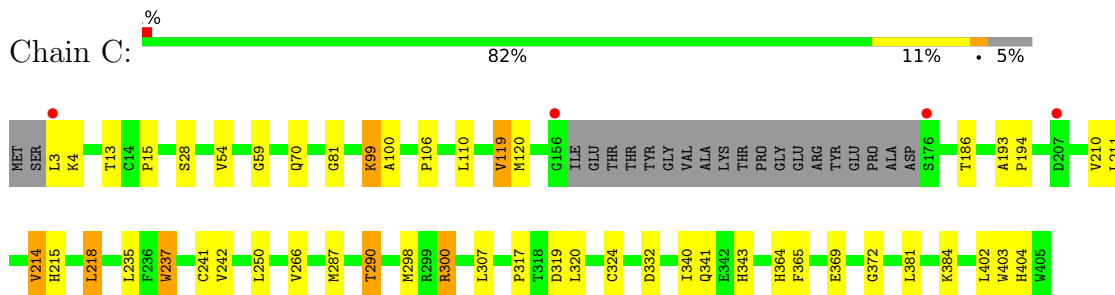
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



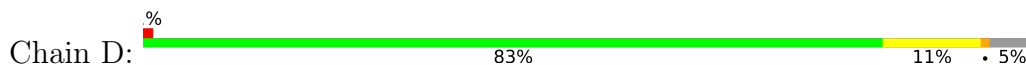
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

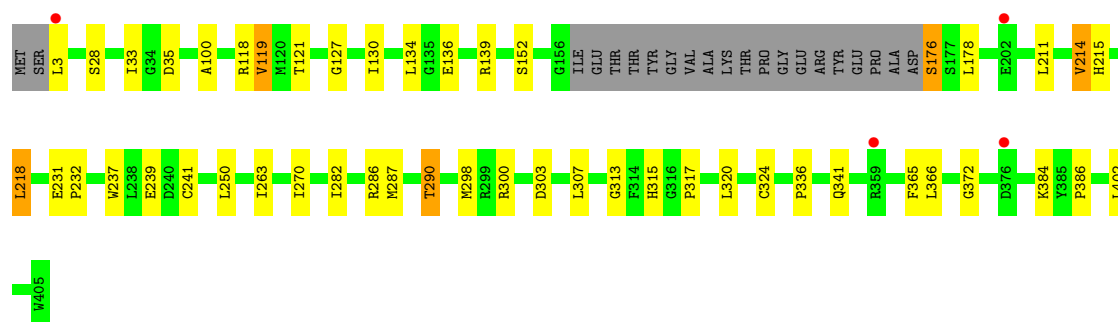


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



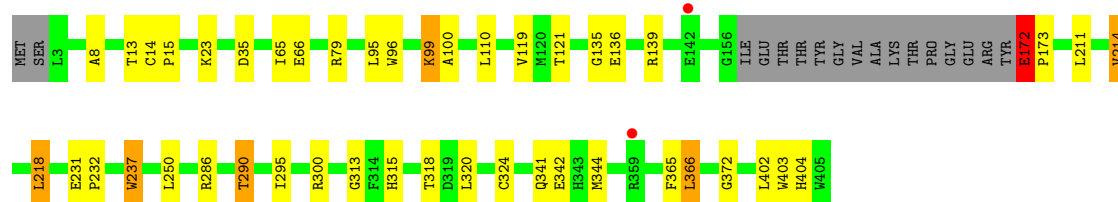
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme





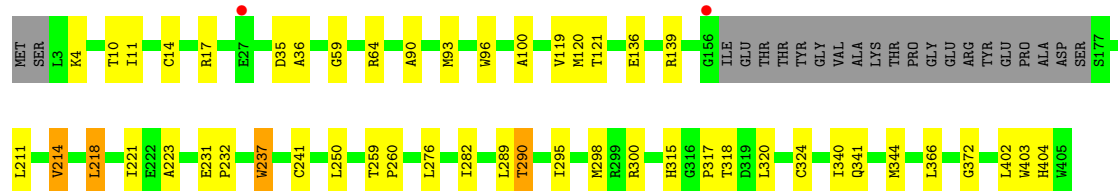
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain E: 84% 10% 6%



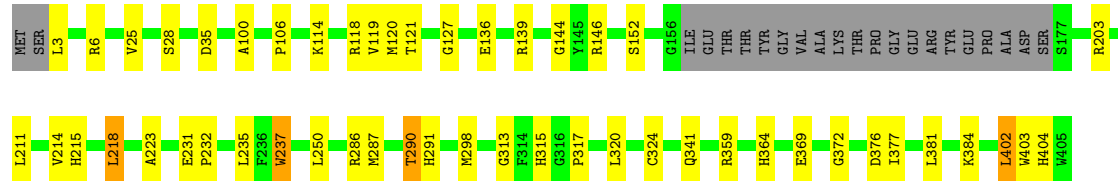
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain F: 82% 11% 7%



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

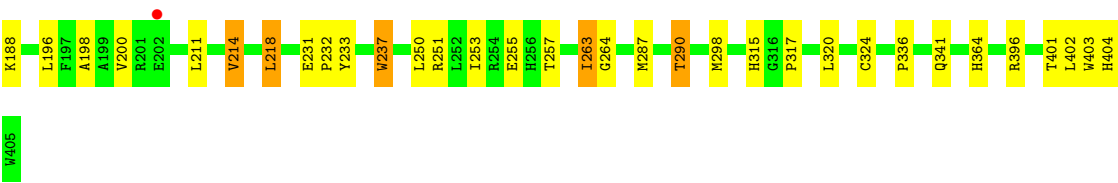
Chain G: 82% 12% 6%



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain H: 82% 11% 7%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.24Å 167.26Å 168.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.82 – 1.80 41.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.82-1.80) 99.8 (41.82-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.199 , 0.241 0.196 , 0.237	Depositor DCC
R_{free} test set	14511 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26363	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KDG, CS2, MG

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	0.47	0/3128	0.79	0/4259
1	B	0.48	0/3158	0.80	2/4301 (0.0%)
1	C	0.47	0/3128	0.78	2/4259 (0.0%)
1	D	0.46	0/3128	0.78	0/4259
1	E	0.49	0/3158	0.80	2/4301 (0.0%)
1	F	0.47	0/3122	0.77	0/4251
1	G	0.46	0/3122	0.77	0/4251
1	H	0.47	0/3122	0.76	0/4251
All	All	0.47	0/25066	0.78	6/34132 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	172	GLU	CA-C-N	7.19	126.72	119.24
1	E	172	GLU	C-N-CA	7.19	126.72	119.24
1	B	81	GLY	CA-C-N	6.86	126.10	118.97
1	B	81	GLY	C-N-CA	6.86	126.10	118.97
1	C	81	GLY	CA-C-N	5.24	124.42	118.97
1	C	81	GLY	C-N-CA	5.24	124.42	118.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3043	0	2936	40	0
1	B	3072	0	2958	35	0
1	C	3043	0	2936	34	0
1	D	3043	0	2936	33	0
1	E	3072	0	2958	30	0
1	F	3037	0	2931	35	0
1	G	3037	0	2931	37	0
1	H	3037	0	2931	32	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	13	0	11	0	0
3	B	13	0	11	0	0
3	E	13	0	10	1	0
3	F	13	0	10	1	0
4	C	12	0	9	0	0
4	D	12	0	9	0	0
4	G	12	0	9	0	0
4	H	12	0	9	0	0
5	A	246	0	0	0	0
5	B	219	0	0	3	0
5	C	233	0	0	4	0
5	D	218	0	0	2	0
5	E	238	0	0	2	0
5	F	237	0	0	1	0
5	G	238	0	0	2	0
5	H	242	0	0	4	0
All	All	26363	0	23595	267	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 6.

All (267) 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:250:LEU:HD22	1:A:276:LEU:HD22	1.34	1.02
1:B:250:LEU:HD22	1:B:276:LEU:HD22	1.53	0.91
1:C:290:THR:HG22	1:C:324:CYS:SG	2.14	0.87
1:F:250:LEU:HD22	1:F:276:LEU:HD22	1.60	0.84
1:D:214:VAL:HG11	1:D:241:CYS:HA	1.58	0.83
1:H:118:ARG:HD2	1:H:364:HIS:CD2	2.15	0.82
1:H:290:THR:HG22	1:H:324:CYS:SG	2.19	0.82
1:D:214:VAL:CG1	1:D:241:CYS:HA	2.11	0.80
1:G:381:LEU:HD12	1:G:384:LYS:HD2	1.65	0.79
1:E:290:THR:HG22	1:E:324:CYS:SG	2.24	0.77
1:C:214:VAL:HG21	1:C:241:CYS:HA	1.66	0.76
1:D:290:THR:HG22	1:D:324:CYS:SG	2.25	0.76
1:D:119:VAL:HG22	1:D:365:PHE:HB2	1.66	0.76
1:A:290:THR:HG22	1:A:324:CYS:SG	2.25	0.76
1:B:290:THR:HG22	1:B:324:CYS:SG	2.25	0.75
1:C:381:LEU:HD12	1:C:384:LYS:HD2	1.71	0.73
1:F:290:THR:HG22	1:F:324:CYS:SG	2.29	0.73
1:D:214:VAL:HG21	1:D:218:LEU:HD22	1.69	0.73
1:D:315:HIS:CE1	1:D:317:PRO:HG3	2.24	0.72
1:C:214:VAL:CG2	1:C:241:CYS:HA	2.19	0.71
1:B:318:THR:HG23	1:B:344:MET:HE2	1.71	0.71
1:H:214:VAL:HG21	1:H:218:LEU:HD22	1.73	0.71
1:B:172:GLU:O	1:B:175:ASP:HB2	1.91	0.71
1:A:250:LEU:HD22	1:A:276:LEU:CD2	2.17	0.71
1:B:119:VAL:HG13	1:B:365:PHE:HB2	1.74	0.70
1:A:290:THR:HG23	1:A:320:LEU:HD22	1.75	0.69
1:D:290:THR:HG23	1:D:320:LEU:HD22	1.72	0.69
1:F:315:HIS:CE1	1:F:317:PRO:HG3	2.25	0.69
1:D:35:ASP:OD2	1:D:290:THR:HG21	1.94	0.67
1:E:214:VAL:HG21	1:E:218:LEU:HD22	1.76	0.67
1:D:136:GLU:OE2	1:D:139:ARG:HD3	1.95	0.66
1:B:136:GLU:HA	1:B:139:ARG:HG2	1.77	0.65
1:H:315:HIS:CE1	1:H:317:PRO:HG3	2.32	0.65
1:A:214:VAL:HG21	1:A:218:LEU:HD22	1.77	0.64
1:B:175:ASP:HB3	5:B:1830:HOH:O	1.99	0.62
1:G:3:LEU:HD13	1:G:28:SER:HB3	1.81	0.62
1:C:290:THR:CG2	1:C:320:LEU:HD22	2.30	0.62
1:F:4:LYS:HE3	1:F:59:GLY:O	1.99	0.62
1:D:3:LEU:HD13	1:D:28:SER:HB3	1.80	0.61
1:F:290:THR:HG23	1:F:320:LEU:HD22	1.81	0.61
1:E:290:THR:HG23	1:E:320:LEU:HD22	1.82	0.60
1:A:35:ASP:OD2	1:A:290:THR:HG21	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:THR:HG23	1:C:320:LEU:HD22	1.81	0.60
1:E:136:GLU:OE2	1:E:139:ARG:HD3	2.02	0.60
1:D:290:THR:CG2	1:D:320:LEU:HD22	2.31	0.59
1:H:263:ILE:HD11	5:H:1388:HOH:O	2.02	0.59
1:H:211:LEU:HD23	1:H:237:TRP:CE2	2.37	0.59
1:H:290:THR:CG2	1:H:324:CYS:SG	2.91	0.59
1:B:359:ARG:HG2	5:B:443:HOH:O	2.01	0.58
1:C:100:ALA:HB3	1:C:372:GLY:HA2	1.85	0.58
1:G:315:HIS:CE1	1:G:317:PRO:HG3	2.38	0.57
1:C:193:ALA:HB3	1:C:194:PRO:HD3	1.85	0.57
1:H:118:ARG:HD2	1:H:364:HIS:CG	2.40	0.57
1:B:218:LEU:O	1:B:242:VAL:HG12	2.04	0.57
1:H:251:ARG:O	1:H:255:GLU:HG3	2.05	0.57
1:B:35:ASP:OD2	1:B:290:THR:HG21	2.05	0.56
1:C:287:MET:HE3	1:C:298:MET:SD	2.45	0.56
1:F:290:THR:CG2	1:F:320:LEU:HD22	2.35	0.56
1:C:4:LYS:HE3	1:C:59:GLY:HA2	1.88	0.56
1:E:100:ALA:HB3	1:E:372:GLY:HA2	1.87	0.55
1:G:136:GLU:HA	1:G:139:ARG:HG2	1.87	0.55
1:G:287:MET:HE3	1:G:298:MET:SD	2.46	0.55
1:F:11:ILE:N	1:F:11:ILE:HD12	2.22	0.55
1:G:403:TRP:CG	1:G:404:HIS:H	2.25	0.55
1:F:315:HIS:NE2	3:F:407:CS2:H3	2.21	0.54
1:G:100:ALA:HB3	1:G:372:GLY:HA2	1.89	0.54
1:F:36:ALA:HB2	1:F:90:ALA:HB2	1.90	0.54
1:B:290:THR:CG2	1:B:324:CYS:SG	2.96	0.54
1:B:295:ILE:O	1:B:299:ARG:HG3	2.08	0.53
1:D:211:LEU:HD23	1:D:237:TRP:CE2	2.44	0.53
1:G:359:ARG:NH2	5:G:1921:HOH:O	2.40	0.53
1:G:290:THR:HG22	1:G:324:CYS:SG	2.48	0.53
1:G:35:ASP:OD2	1:G:290:THR:HG21	2.08	0.53
1:F:136:GLU:HA	1:F:139:ARG:HG2	1.91	0.53
1:D:136:GLU:HA	1:D:139:ARG:HG2	1.91	0.53
1:G:144:GLY:O	1:G:146:ARG:NH1	2.41	0.52
1:A:211:LEU:HD23	1:A:237:TRP:CE2	2.44	0.52
1:F:35:ASP:OD2	1:F:290:THR:HG21	2.09	0.52
1:A:3:LEU:HD13	1:A:28:SER:HB3	1.91	0.52
1:A:290:THR:CG2	1:A:320:LEU:HD22	2.39	0.52
1:G:120:MET:HA	1:G:364:HIS:CD2	2.45	0.52
1:C:3:LEU:CD1	1:C:28:SER:HB3	2.40	0.52
1:F:218:LEU:HD23	1:F:223:ALA:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:LEU:O	1:H:200:VAL:HG23	2.11	0.51
1:A:295:ILE:O	1:A:299:ARG:HG3	2.10	0.51
1:B:100:ALA:HB3	1:B:372:GLY:HA2	1.92	0.51
1:E:366:LEU:N	1:E:366:LEU:HD22	2.26	0.51
1:A:136:GLU:HA	1:A:139:ARG:HG2	1.92	0.51
1:B:359:ARG:HG3	1:B:366:LEU:HB2	1.93	0.51
1:C:364:HIS:HB2	5:C:526:HOH:O	2.11	0.51
1:E:290:THR:CG2	1:E:320:LEU:HD22	2.41	0.51
1:E:14:CYS:N	1:E:15:PRO:HD3	2.25	0.51
1:H:187:GLU:CD	5:H:792:HOH:O	2.52	0.51
1:A:403:TRP:CG	1:A:404:HIS:H	2.28	0.50
1:B:315:HIS:CE1	1:B:317:PRO:HG3	2.46	0.50
1:D:33:ILE:HG23	5:D:1944:HOH:O	2.11	0.50
1:C:13:THR:HG23	1:C:15:PRO:HD3	1.94	0.50
1:H:287:MET:HE3	1:H:298:MET:SD	2.52	0.50
1:A:124:HIS:CE1	1:A:344:MET:SD	3.05	0.50
1:C:211:LEU:HD12	1:C:211:LEU:N	2.27	0.50
1:D:121:THR:HA	1:D:341:GLN:O	2.12	0.50
1:G:203:ARG:HD3	5:G:1548:HOH:O	2.11	0.50
1:H:263:ILE:HD13	1:H:264:GLY:N	2.27	0.50
1:H:136:GLU:HA	1:H:139:ARG:HG2	1.94	0.50
1:F:10:THR:C	1:F:11:ILE:HD12	2.37	0.50
1:A:270:ILE:HD13	1:D:307:LEU:HD21	1.93	0.50
1:E:318:THR:HG23	1:E:344:MET:HE2	1.93	0.50
1:G:136:GLU:OE2	1:G:139:ARG:HD3	2.10	0.49
1:G:376:ASP:CG	1:G:377:ILE:H	2.18	0.49
1:A:9:TYR:OH	1:A:23:LYS:HD3	2.11	0.49
1:D:127:GLY:O	1:D:152:SER:HA	2.12	0.49
1:F:120:MET:HE3	1:F:340:ILE:HD12	1.93	0.49
1:G:376:ASP:OD1	1:G:377:ILE:N	2.40	0.49
1:A:250:LEU:HD23	1:A:282:ILE:HG23	1.95	0.49
1:C:266:VAL:HG22	5:C:1106:HOH:O	2.12	0.49
1:C:332:ASP:OD2	1:C:341:GLN:NE2	2.45	0.49
1:D:287:MET:HE3	1:D:298:MET:SD	2.53	0.48
1:E:403:TRP:CG	1:E:404:HIS:H	2.30	0.48
1:H:403:TRP:CG	1:H:404:HIS:H	2.31	0.48
1:E:121:THR:HA	1:E:341:GLN:O	2.12	0.48
1:G:376:ASP:CG	1:G:377:ILE:N	2.72	0.48
1:A:250:LEU:HD23	1:A:282:ILE:CG2	2.43	0.48
1:D:214:VAL:HG12	1:D:239:GLU:O	2.13	0.48
1:F:290:THR:CG2	1:F:324:CYS:SG	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:LEU:CD1	1:G:28:SER:HB3	2.43	0.48
1:C:300:ARG:NH1	5:C:1925:HOH:O	2.42	0.48
1:A:13:THR:HG23	1:A:15:PRO:HD3	1.95	0.47
1:C:3:LEU:HD13	1:C:28:SER:HB3	1.96	0.47
1:C:120:MET:HE3	1:C:340:ILE:HD12	1.97	0.47
1:C:237:TRP:CD1	1:C:237:TRP:C	2.92	0.47
1:G:211:LEU:HD23	1:G:237:TRP:CE2	2.49	0.47
1:B:119:VAL:HG23	1:B:338:PHE:CZ	2.48	0.47
1:G:290:THR:CG2	1:G:324:CYS:SG	3.03	0.47
1:A:280:GLN:HB3	1:B:252:LEU:HD11	1.97	0.47
1:B:290:THR:HG23	1:B:320:LEU:HD22	1.96	0.47
1:H:237:TRP:CD1	1:H:237:TRP:C	2.91	0.47
1:E:13:THR:C	1:E:15:PRO:HD3	2.39	0.47
1:B:211:LEU:HD23	1:B:237:TRP:CE2	2.49	0.47
1:G:235:LEU:HD12	1:G:235:LEU:N	2.30	0.47
1:G:237:TRP:CD1	1:G:237:TRP:C	2.93	0.47
1:B:123:ALA:HB2	1:B:145:TYR:CD2	2.49	0.47
1:F:237:TRP:CD1	1:F:237:TRP:C	2.92	0.47
1:D:214:VAL:HG13	1:D:241:CYS:HA	1.93	0.47
1:F:14:CYS:HA	1:F:17:ARG:O	2.15	0.47
1:F:318:THR:HG23	1:F:344:MET:HE2	1.97	0.46
1:H:121:THR:HA	1:H:341:GLN:O	2.14	0.46
1:F:64:ARG:NH1	1:G:114:LYS:HE3	2.30	0.46
1:G:6:ARG:HH21	1:G:25:VAL:HG11	1.80	0.46
1:C:343:HIS:CD2	1:C:365:PHE:HZ	2.33	0.46
1:B:214:VAL:HG22	1:B:241:CYS:HA	1.98	0.46
1:G:214:VAL:HG11	1:G:218:LEU:HD22	1.96	0.46
1:H:142:GLU:HB3	5:H:1292:HOH:O	2.16	0.46
1:A:211:LEU:HD12	1:A:211:LEU:N	2.31	0.45
1:H:35:ASP:OD2	1:H:290:THR:HG21	2.17	0.45
1:A:307:LEU:HD21	1:D:270:ILE:HD13	1.97	0.45
1:C:317:PRO:HB2	1:C:319:ASP:OD1	2.16	0.45
1:A:218:LEU:O	1:A:242:VAL:HG12	2.16	0.45
1:B:231:GLU:N	1:B:232:PRO:CD	2.80	0.45
1:B:403:TRP:CG	1:B:404:HIS:H	2.35	0.45
1:E:365:PHE:C	1:E:366:LEU:HD22	2.41	0.45
1:D:130:ILE:O	1:D:134:LEU:HG	2.16	0.45
1:F:121:THR:HA	1:F:341:GLN:O	2.17	0.45
1:A:66:GLU:CD	1:A:300:ARG:HH22	2.24	0.45
1:A:66:GLU:OE2	1:D:336:PRO:HG3	2.17	0.45
1:A:315:HIS:CE1	1:A:317:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:HIS:NE2	3:E:407:CS2:H3	2.32	0.44
1:B:237:TRP:CD1	1:B:237:TRP:C	2.95	0.44
1:E:99:LYS:HG2	1:E:110:LEU:HD21	2.00	0.44
1:A:193:ALA:HB3	1:A:194:PRO:HD3	1.98	0.44
1:G:381:LEU:HA	1:G:384:LYS:HD2	1.99	0.44
1:H:290:THR:HG23	1:H:320:LEU:HD22	1.99	0.44
1:B:123:ALA:HB2	1:B:145:TYR:CE2	2.52	0.44
1:A:187:GLU:OE2	1:A:191:ASN:ND2	2.50	0.44
1:A:213:ASP:HA	1:A:239:GLU:HB3	1.99	0.44
1:G:290:THR:CG2	1:G:324:CYS:HB2	2.48	0.44
1:G:218:LEU:HD23	1:G:223:ALA:HA	1.99	0.44
1:C:99:LYS:HG2	1:C:110:LEU:HD21	1.99	0.43
1:C:119:VAL:HG22	1:C:365:PHE:HB2	1.99	0.43
1:F:231:GLU:N	1:F:232:PRO:CD	2.81	0.43
1:G:211:LEU:N	1:G:211:LEU:HD12	2.33	0.43
1:A:100:ALA:HB3	1:A:372:GLY:HA2	1.99	0.43
1:B:270:ILE:HD13	1:C:307:LEU:HD21	1.99	0.43
1:E:290:THR:CG2	1:E:324:CYS:SG	3.00	0.43
1:F:93:MET:HE3	1:F:93:MET:HB2	1.87	0.43
1:A:121:THR:HA	1:A:341:GLN:O	2.18	0.43
1:D:136:GLU:CD	1:D:139:ARG:HD3	2.42	0.43
1:E:342:GLU:N	5:E:1073:HOH:O	2.51	0.43
1:G:290:THR:HG22	1:G:324:CYS:HB2	2.01	0.43
1:A:65:ILE:HG12	1:A:95:LEU:HB3	2.00	0.43
1:F:214:VAL:HG22	1:F:241:CYS:HA	2.01	0.43
1:C:290:THR:HG21	1:C:320:LEU:HD22	2.01	0.43
1:E:237:TRP:CD1	1:E:237:TRP:C	2.97	0.43
1:F:403:TRP:CG	1:F:404:HIS:H	2.35	0.43
1:H:198:ALA:HB2	1:H:233:TYR:CZ	2.53	0.43
1:G:106:PRO:HG3	1:G:369:GLU:O	2.18	0.43
1:G:127:GLY:O	1:G:152:SER:HA	2.18	0.43
1:C:106:PRO:HG3	1:C:369:GLU:O	2.19	0.43
1:F:100:ALA:HB3	1:F:372:GLY:HA2	2.00	0.43
1:C:214:VAL:HG22	1:C:241:CYS:HA	1.98	0.43
1:E:135:GLY:O	1:E:139:ARG:HG2	2.19	0.42
1:E:231:GLU:N	1:E:232:PRO:CD	2.82	0.42
1:F:96:TRP:CD1	1:F:295:ILE:HB	2.54	0.42
1:H:253:ILE:O	1:H:257:THR:HG22	2.19	0.42
1:E:35:ASP:OD2	1:E:290:THR:HG21	2.18	0.42
1:E:65:ILE:HG12	1:E:95:LEU:HB3	2.00	0.42
1:E:66:GLU:CD	1:H:336:PRO:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:ARG:NH1	5:F:767:HOH:O	2.39	0.42
1:H:231:GLU:N	1:H:232:PRO:CD	2.82	0.42
1:H:79:ARG:O	1:H:80:ARG:HB2	2.20	0.42
1:F:211:LEU:HD12	1:F:211:LEU:N	2.33	0.42
1:A:230:VAL:HB	1:A:235:LEU:HD11	2.00	0.42
1:B:138:ALA:O	1:B:142:GLU:HG2	2.20	0.42
1:H:396:ARG:HA	1:H:401:THR:O	2.20	0.42
1:B:124:HIS:CE1	1:B:344:MET:SD	3.13	0.42
1:E:96:TRP:CD1	1:E:295:ILE:HB	2.54	0.42
1:F:289:LEU:HD23	1:F:298:MET:HG3	2.02	0.42
1:G:121:THR:HA	1:G:341:GLN:O	2.19	0.42
1:G:286:ARG:HD2	1:G:313:GLY:O	2.20	0.42
1:C:403:TRP:CG	1:C:404:HIS:H	2.37	0.42
1:D:286:ARG:HD2	1:D:313:GLY:O	2.20	0.42
1:A:123:ALA:HB2	1:A:145:TYR:CD2	2.55	0.42
1:B:286:ARG:HD2	1:B:313:GLY:O	2.20	0.42
1:E:8:ALA:HA	1:E:23:LYS:O	2.20	0.42
1:E:172:GLU:HA	1:E:173:PRO:HD3	1.74	0.42
1:D:231:GLU:N	1:D:232:PRO:CD	2.82	0.41
1:E:66:GLU:CD	1:E:300:ARG:HH22	2.28	0.41
1:E:211:LEU:HD23	1:E:237:TRP:CE2	2.54	0.41
1:F:250:LEU:HD23	1:F:282:ILE:CG2	2.49	0.41
1:F:259:THR:HA	1:F:260:PRO:HD3	1.97	0.41
1:G:231:GLU:N	1:G:232:PRO:CD	2.83	0.41
1:D:384:LYS:O	1:D:386:PRO:HD3	2.20	0.41
1:A:136:GLU:OE2	1:A:139:ARG:HD3	2.20	0.41
1:B:218:LEU:HG	1:B:222:GLU:HB3	2.03	0.41
1:C:211:LEU:HD23	1:C:237:TRP:CE2	2.55	0.41
1:C:186:THR:HG23	1:C:218:LEU:HD12	2.02	0.41
1:A:303:ASP:OD2	1:D:303:ASP:OD2	2.37	0.41
1:C:70:GLN:C	1:G:402:LEU:HD22	2.46	0.41
1:D:100:ALA:HB3	1:D:372:GLY:HA2	2.02	0.41
1:H:185:SER:OG	1:H:188:LYS:HG3	2.20	0.41
1:B:173:PRO:HD2	5:B:1951:HOH:O	2.20	0.41
1:F:289:LEU:HD22	1:F:295:ILE:HD13	2.03	0.41
1:H:124:HIS:CE1	1:H:149:ARG:CZ	3.04	0.41
1:B:300:ARG:HB3	5:C:858:HOH:O	2.20	0.41
1:A:286:ARG:HD2	1:A:313:GLY:O	2.20	0.41
1:B:121:THR:HA	1:B:341:GLN:O	2.21	0.41
1:B:322:PRO:HG2	1:B:354:PHE:HB2	2.02	0.41
1:C:210:VAL:C	1:C:211:LEU:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ARG:HA	5:E:557:HOH:O	2.20	0.41
1:E:286:ARG:HD2	1:E:313:GLY:O	2.20	0.41
1:F:221:ILE:HD12	1:F:221:ILE:HA	1.87	0.41
1:F:366:LEU:HD22	1:F:366:LEU:N	2.36	0.41
1:H:6:ARG:HH21	1:H:25:VAL:HG11	1.86	0.41
1:A:136:GLU:CD	1:A:139:ARG:HD3	2.46	0.41
1:C:218:LEU:O	1:C:242:VAL:HG12	2.21	0.41
1:D:237:TRP:CD1	1:D:237:TRP:C	2.99	0.41
1:F:211:LEU:HD23	1:F:237:TRP:CE2	2.56	0.41
1:A:120:MET:HA	1:A:364:HIS:CD2	2.56	0.40
1:B:127:GLY:O	1:B:152:SER:HA	2.21	0.40
1:D:300:ARG:NH1	5:D:768:HOH:O	2.44	0.40
1:A:93:MET:SD	1:A:323:VAL:HG12	2.61	0.40
1:H:14:CYS:HA	1:H:17:ARG:O	2.21	0.40
1:H:42:GLU:HA	5:H:435:HOH:O	2.20	0.40
1:A:235:LEU:HD12	1:A:235:LEU:N	2.36	0.40
1:D:176:SER:HB3	1:D:178:LEU:O	2.21	0.40
1:D:263:ILE:HG22	1:D:282:ILE:HG21	2.03	0.40
1:H:290:THR:CG2	1:H:320:LEU:HD22	2.51	0.40
1:G:291:HIS:CE1	1:G:320:LEU:HD21	2.56	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	380/405 (94%)	370 (97%)	10 (3%)	0	100	100
1	B	384/405 (95%)	371 (97%)	13 (3%)	0	100	100
1	C	380/405 (94%)	371 (98%)	9 (2%)	0	100	100
1	D	380/405 (94%)	370 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	384/405 (95%)	372 (97%)	12 (3%)	0	100	100
1	F	379/405 (94%)	367 (97%)	12 (3%)	0	100	100
1	G	379/405 (94%)	368 (97%)	11 (3%)	0	100	100
1	H	379/405 (94%)	364 (96%)	15 (4%)	0	100	100
All	All	3045/3240 (94%)	2953 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	315/332 (95%)	307 (98%)	8 (2%)	42	30
1	B	318/332 (96%)	313 (98%)	5 (2%)	55	47
1	C	315/332 (95%)	303 (96%)	12 (4%)	29	17
1	D	315/332 (95%)	305 (97%)	10 (3%)	34	22
1	E	318/332 (96%)	308 (97%)	10 (3%)	35	23
1	F	314/332 (95%)	308 (98%)	6 (2%)	50	41
1	G	314/332 (95%)	306 (98%)	8 (2%)	42	30
1	H	314/332 (95%)	306 (98%)	8 (2%)	42	30
All	All	2523/2656 (95%)	2456 (97%)	67 (3%)	39	27

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	119	VAL
1	A	214	VAL
1	A	215	HIS
1	A	218	LEU
1	A	290	THR

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Mol	Chain	Res	Type
1	A	366	LEU
1	A	402	LEU
1	B	119	VAL
1	B	214	VAL
1	B	218	LEU
1	B	237	TRP
1	B	290	THR
1	C	54	VAL
1	C	99	LYS
1	C	119	VAL
1	C	214	VAL
1	C	215	HIS
1	C	218	LEU
1	C	235	LEU
1	C	237	TRP
1	C	250	LEU
1	C	290	THR
1	C	300	ARG
1	C	402	LEU
1	D	118	ARG
1	D	119	VAL
1	D	176	SER
1	D	214	VAL
1	D	215	HIS
1	D	218	LEU
1	D	250	LEU
1	D	290	THR
1	D	366	LEU
1	D	402	LEU
1	E	99	LYS
1	E	119	VAL
1	E	172	GLU
1	E	214	VAL
1	E	218	LEU
1	E	237	TRP
1	E	250	LEU
1	E	290	THR
1	E	366	LEU
1	E	402	LEU
1	F	119	VAL
1	F	214	VAL
1	F	218	LEU

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Mol	Chain	Res	Type
1	F	237	TRP
1	F	290	THR
1	F	402	LEU
1	G	118	ARG
1	G	119	VAL
1	G	215	HIS
1	G	218	LEU
1	G	237	TRP
1	G	250	LEU
1	G	290	THR
1	G	402	LEU
1	H	119	VAL
1	H	214	VAL
1	H	218	LEU
1	H	237	TRP
1	H	250	LEU
1	H	263	ILE
1	H	290	THR
1	H	402	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	B	192	HIS
1	B	234	HIS
1	D	234	HIS
1	E	192	HIS
1	E	234	HIS
1	E	278	GLN
1	F	234	HIS
1	F	341	GLN
1	G	234	HIS
1	G	280	GLN
1	H	280	GLN
1	H	364	HIS

5.3.3 RNA ⓘ

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	CS2	E	407	2	12,12,12	0.72	0	15,16,16	1.38	2 (13%)
4	KDG	D	407	2	11,11,11	0.92	1 (9%)	13,14,14	1.59	3 (23%)
3	CS2	F	407	2	12,12,12	0.63	0	15,16,16	1.11	2 (13%)
4	KDG	G	407	2	11,11,11	1.05	1 (9%)	13,14,14	1.60	3 (23%)
3	CS2	B	407	2	12,12,12	0.56	0	15,16,16	0.93	0
3	CS2	A	407	2	12,12,12	0.59	0	15,16,16	1.21	2 (13%)
4	KDG	H	407	2	11,11,11	0.83	1 (9%)	13,14,14	1.49	3 (23%)
4	KDG	C	407	2	11,11,11	0.88	1 (9%)	13,14,14	2.35	5 (38%)

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	CS2	E	407	2	-	1/18/18/18	-
4	KDG	D	407	2	-	0/14/14/14	-
3	CS2	F	407	2	-	3/18/18/18	-
4	KDG	G	407	2	-	0/14/14/14	-
3	CS2	B	407	2	-	5/18/18/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CS2	A	407	2	-	6/18/18/18	-
4	KDG	H	407	2	-	0/14/14/14	-
4	KDG	C	407	2	-	2/14/14/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	407	KDG	C5-C6	-3.00	1.49	1.53
4	D	407	KDG	C5-C6	-2.36	1.49	1.53
4	C	407	KDG	C5-C6	-2.10	1.50	1.53
4	H	407	KDG	C5-C6	-2.00	1.50	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	407	KDG	C4-C3-C2	-4.68	105.55	113.55
4	C	407	KDG	O6A-C6-C5	3.90	124.40	113.59
4	C	407	KDG	O5-C5-C6	3.43	124.56	119.67
4	G	407	KDG	C4-C3-C2	-3.35	107.83	113.55
4	D	407	KDG	C4-C3-C2	-3.24	108.02	113.55
4	H	407	KDG	C4-C3-C2	-3.22	108.05	113.55
3	E	407	CS2	C5-C4-C3	-3.13	107.67	112.48
3	A	407	CS2	C5-C4-C3	-2.92	108.00	112.48
4	C	407	KDG	O6A-C6-O6B	-2.82	117.19	123.90
3	F	407	CS2	O1A-C1-O1B	-2.81	117.71	124.08
4	G	407	KDG	O6A-C6-C5	2.77	121.28	113.59
4	H	407	KDG	O6A-C6-C5	2.76	121.25	113.59
4	D	407	KDG	O6A-C6-C5	2.74	121.20	113.59
4	C	407	KDG	O6B-C6-C5	-2.73	118.42	121.81
4	H	407	KDG	O6A-C6-O6B	-2.70	117.46	123.90
3	A	407	CS2	O1A-C1-O1B	-2.37	118.71	124.08
3	E	407	CS2	O1A-C1-O1B	-2.33	118.80	124.08
4	D	407	KDG	O6A-C6-O6B	-2.28	118.47	123.90
3	F	407	CS2	O1A-C1-C2	2.19	119.40	113.31
4	G	407	KDG	O6A-C6-O6B	-2.02	119.08	123.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	407	CS2	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	C	407	KDG	C4-C5-C6-O6A
3	B	407	CS2	O2-C2-C3-O3
3	A	407	CS2	O4-C4-C5-C6
3	A	407	CS2	O2-C2-C3-O3
3	A	407	CS2	O2-C2-C3-C4
4	C	407	KDG	O2-C2-C3-O3
3	F	407	CS2	C3-C4-C5-O5
3	A	407	CS2	O4-C4-C5-O5
3	E	407	CS2	O4-C4-C5-C6
3	F	407	CS2	O4-C4-C5-C6
3	A	407	CS2	C3-C4-C5-O5
3	F	407	CS2	O4-C4-C5-O5
3	A	407	CS2	C3-C4-C5-C6
3	B	407	CS2	C1-C2-C3-O3
3	B	407	CS2	C1-C2-C3-C4
3	B	407	CS2	O4-C4-C5-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	407	CS2	1	0
3	F	407	CS2	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	384/405 (94%)	-0.01	2 (0%) 87 88	14, 18, 30, 40	0
1	B	388/405 (95%)	-0.04	4 (1%) 79 80	14, 18, 30, 44	0
1	C	384/405 (94%)	0.06	4 (1%) 79 80	13, 19, 30, 39	0
1	D	384/405 (94%)	-0.06	4 (1%) 79 80	13, 19, 30, 38	0
1	E	388/405 (95%)	-0.06	2 (0%) 87 88	13, 18, 29, 40	0
1	F	383/405 (94%)	0.00	2 (0%) 87 88	13, 19, 31, 40	0
1	G	383/405 (94%)	-0.03	0 100 100	13, 18, 30, 40	0
1	H	383/405 (94%)	-0.00	2 (0%) 87 88	13, 18, 29, 42	0
All	All	3077/3240 (94%)	-0.02	20 (0%) 85 86	13, 18, 30, 44	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	156	GLY	3.6
1	C	3	LEU	3.4
1	C	156	GLY	3.1
1	C	176	SER	3.1
1	D	202	GLU	2.9
1	B	156	GLY	2.8
1	B	141	VAL	2.8
1	C	207	ASP	2.8
1	F	156	GLY	2.6
1	F	27	GLU	2.6
1	H	202	GLU	2.4
1	E	359	ARG	2.4
1	A	176	SER	2.4
1	B	207	ASP	2.3
1	D	359	ARG	2.3
1	D	376	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	207	ASP	2.1
1	D	3	LEU	2.1
1	B	175	ASP	2.1
1	E	142	GLU	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
3	CS2	A	407	13/13	0.89	0.11	16,22,28,31	0
3	CS2	F	407	13/13	0.90	0.10	19,22,29,31	0
4	KDG	D	407	12/12	0.90	0.09	16,21,28,30	0
4	KDG	G	407	12/12	0.90	0.09	19,20,26,26	0
4	KDG	C	407	12/12	0.92	0.09	15,22,25,28	0
3	CS2	E	407	13/13	0.92	0.09	15,19,27,33	0
3	CS2	B	407	13/13	0.92	0.09	13,22,27,28	0
4	KDG	H	407	12/12	0.92	0.08	14,19,22,27	0
2	MG	E	406	1/1	0.97	0.03	19,19,19,19	0
2	MG	H	406	1/1	0.98	0.03	17,17,17,17	0
2	MG	D	406	1/1	0.98	0.02	18,18,18,18	0
2	MG	B	406	1/1	0.98	0.08	18,18,18,18	0
2	MG	A	406	1/1	0.99	0.03	17,17,17,17	0
2	MG	F	406	1/1	0.99	0.04	19,19,19,19	0
2	MG	G	406	1/1	0.99	0.03	19,19,19,19	0
2	MG	C	406	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.