



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:51 AM UTC

PDB ID : 3ZPH / pdb_00003zph
Title : Bacterial chalcone isomerase in closed conformation from Eubacterium ramulus at 2.8 Å resolution
Authors : Thomsen, M.; Palm, G.J.; Hinrichs, W.
Deposited on : 2013-02-27
Resolution : 2.80 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

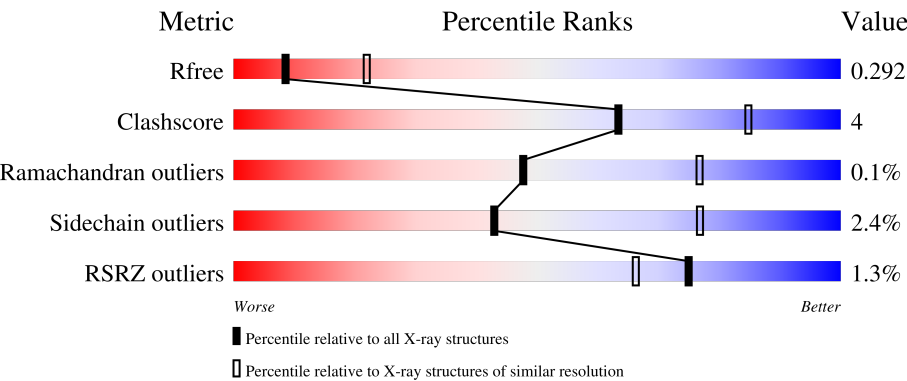
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	282	% 82%10%8%
1	B	282	2% 90%9%
1	C	282	% 78%13%9%
1	D	282	% 82%10%9%
1	E	282	% 80%11%9%

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Mol	Chain	Length	Quality of chain
1	F	282	% 80% 10% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14021 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 CHALCONE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2132	1392	347	380	13			
1	B	282	Total	C	N	O	S	0	0	0
			2287	1478	379	417	13			
1	C	258	Total	C	N	O	S	0	1	0
			2125	1388	345	379	13			
1	D	258	Total	C	N	O	S	0	2	0
			2131	1392	345	381	13			
1	E	258	Total	C	N	O	S	0	1	0
			2125	1388	345	379	13			
1	F	258	Total	C	N	O	S	0	1	0
			2125	1388	345	379	13			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

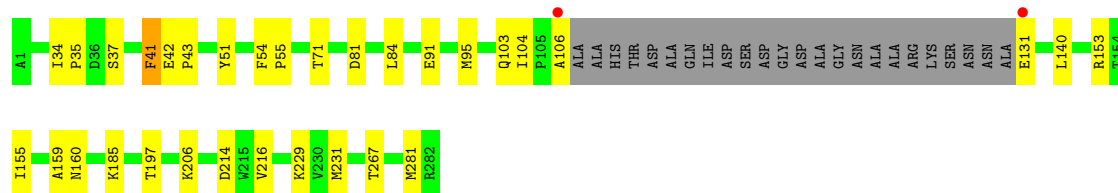
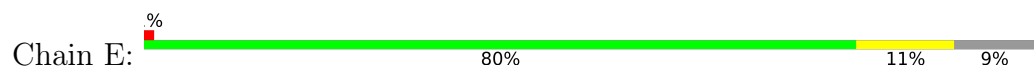
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

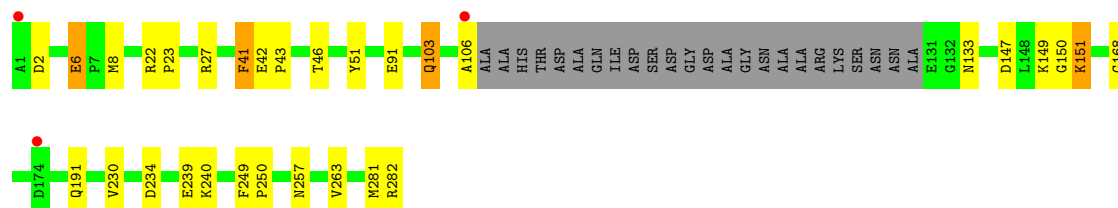
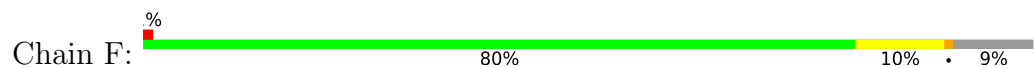
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	214	Total O 215 215	0	1
4	B	196	Total O 196 196	0	0
4	C	177	Total O 177 177	0	0
4	D	163	Total O 163 163	0	0
4	E	144	Total O 144 144	0	0
4	F	167	Total O 167 167	0	0

- Molecule 1: CHALCONE ISOMERASE



- Molecule 1: CHALCONE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	177.73Å 203.12Å 206.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.09 – 2.80 20.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.09-2.80) 99.0 (20.09-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.248 , 0.297 0.250 , 0.292	Depositor DCC
R_{free} test set	4539 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14021	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: CL, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.88	1/2203 (0.0%)	0.97	4/2995 (0.1%)
1	B	0.90	2/2360 (0.1%)	0.96	0/3209
1	C	0.86	0/2199	0.95	6/2989 (0.2%)
1	D	0.86	0/2208	0.89	2/3001 (0.1%)
1	E	0.88	0/2199	0.96	3/2989 (0.1%)
1	F	0.85	0/2199	0.92	1/2989 (0.0%)
All	All	0.87	3/13368 (0.0%)	0.94	16/18172 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	HIS	CG-CD2	5.62	1.42	1.35
1	B	143	TRP	CA-C	-5.44	1.46	1.52
1	B	109	HIS	CG-CD2	5.28	1.41	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	LYS	CA-C-N	-7.68	112.76	120.98
1	C	240	LYS	C-N-CA	-7.68	112.76	120.98
1	A	208	ILE	N-CA-C	6.33	116.50	110.42
1	C	40	GLN	N-CA-C	6.08	117.58	111.07
1	F	41	PHE	N-CA-C	5.65	120.16	112.88
1	E	41	PHE	N-CA-C	5.63	120.14	112.88
1	C	140	LEU	CA-C-N	-5.62	114.46	120.03
1	C	140	LEU	C-N-CA	-5.62	114.46	120.03
1	D	158	GLY	N-CA-C	5.54	117.67	112.08
1	A	22	ARG	CA-C-N	-5.53	113.02	119.32
1	A	22	ARG	C-N-CA	-5.53	113.02	119.32
1	E	231	MET	CA-C-N	-5.38	117.70	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	231	MET	C-N-CA	-5.38	117.70	122.97
1	C	69	GLN	N-CA-C	5.25	116.27	108.60
1	D	224	GLN	N-CA-C	5.22	116.65	111.07
1	A	132	GLY	N-CA-C	5.06	118.12	111.03

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	2132	0	2062	14	0
1	B	2287	0	2197	20	0
1	C	2125	0	2057	24	0
1	D	2131	0	2063	19	0
1	E	2125	0	2057	15	0
1	F	2125	0	2057	21	0
2	A	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	2	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	215	0	0	6	0
4	B	196	0	0	5	0
4	C	177	0	0	3	0
4	D	163	0	0	3	0
4	E	144	0	0	1	0
4	F	167	0	0	2	0
All	All	14021	0	12533	102	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 4.

All (102) 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:C:263:VAL:CG2	1:F:281:MET:HE1	2.14	0.77
1:B:85:GLU:HG2	4:B:2077:HOH:O	1.88	0.74
1:C:263:VAL:HG21	1:F:281:MET:HE1	1.70	0.72
1:B:108:ALA:O	1:B:109:HIS:CD2	2.45	0.70
1:C:281:MET:HE3	1:F:51:TYR:CD1	2.28	0.69
1:C:7:PRO:CB	1:C:142:MET:HE3	2.24	0.68
1:A:183:PHE:CE2	4:A:2174:HOH:O	2.48	0.67
1:A:266:TYR:OH	4:A:2201:HOH:O	2.11	0.67
1:A:182:LEU:HD23	4:A:2174:HOH:O	1.94	0.66
1:D:106:ALA:C	4:D:2074:HOH:O	2.41	0.63
1:A:167:ILE:HD11	1:A:182:LEU:HD22	1.81	0.63
1:E:206:LYS:CE	1:E:214:ASP:OD1	2.48	0.62
1:E:206:LYS:HE2	1:E:214:ASP:OD1	2.01	0.61
1:F:6:GLU:HG2	1:F:8:MET:HE2	1.84	0.58
1:C:206:LYS:HE3	1:C:213:MET:O	2.04	0.58
1:D:135:PHE:HE1	2:D:401:GOL:HO1	1.50	0.58
1:D:131:GLU:N	4:D:2078:HOH:O	2.38	0.57
1:F:106:ALA:C	4:F:2066:HOH:O	2.47	0.57
1:C:7:PRO:HB2	1:C:142:MET:HE3	1.87	0.56
1:E:81:ASP:HB3	1:E:84:LEU:HD13	1.88	0.56
1:E:106:ALA:C	4:E:2071:HOH:O	2.48	0.56
1:C:263:VAL:HG23	1:F:281:MET:HE1	1.88	0.56
1:D:135:PHE:HE1	2:D:401:GOL:O1	1.89	0.56
1:A:14:VAL:O	1:A:66:ALA:HB1	2.08	0.54
4:C:2048:HOH:O	1:F:282:ARG:HG3	2.08	0.54
1:C:15:ASP:HB2	4:C:2019:HOH:O	2.08	0.53
1:C:281:MET:HE3	1:F:51:TYR:CG	2.45	0.52
1:E:206:LYS:HE3	1:E:214:ASP:OD1	2.11	0.50
1:B:146:LYS:HE3	4:B:2116:HOH:O	2.12	0.50
1:D:106:ALA:C	4:D:2073:HOH:O	2.53	0.50
1:A:182:LEU:HD21	1:A:217:LEU:HD11	1.93	0.50
1:B:108:ALA:O	1:B:109:HIS:CG	2.64	0.50
1:B:195:GLU:HG3	4:B:2069:HOH:O	2.12	0.49
1:F:249:PHE:CG	1:F:250:PRO:HA	2.47	0.49
1:C:281:MET:HE1	1:F:263:VAL:HG21	1.94	0.49
1:E:34:ILE:HB	1:E:35:PRO:HD3	1.94	0.49
1:F:22:ARG:HB3	1:F:23:PRO:HD3	1.95	0.49
1:B:1:ALA:HB1	4:B:2003:HOH:O	2.12	0.49
1:C:239:GLU:HG2	4:C:2069:HOH:O	2.12	0.48
1:F:168:GLY:O	1:F:257:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLN:HA	1:C:133:ASN:O	2.13	0.48
1:E:42:GLU:HB3	1:E:43:PRO:HD3	1.95	0.48
1:E:51:TYR:CE2	1:E:267:THR:HG22	2.49	0.48
1:C:249:PHE:CD1	1:C:250:PRO:HA	2.49	0.48
1:A:51:TYR:CG	1:E:281:MET:HE3	2.49	0.48
1:B:41:PHE:CD1	1:B:45:VAL:HB	2.49	0.48
1:B:91:GLU:OE2	1:B:121:GLY:HA3	2.15	0.47
1:C:149:LYS:O	1:C:198:ARG:HA	2.14	0.47
1:A:205:LYS:HE2	4:A:2168:HOH:O	2.14	0.47
1:C:159:ALA:HB2	1:F:27:ARG:HD2	1.96	0.46
1:F:42:GLU:N	1:F:43:PRO:CD	2.79	0.46
1:A:7:PRO:HA	1:A:75:TRP:O	2.16	0.46
1:A:27:ARG:HD2	1:E:159:ALA:HB2	1.98	0.46
1:D:17:VAL:HG11	1:D:102:GLY:HA3	1.97	0.46
1:D:182:LEU:HD23	1:D:183:PHE:CE2	2.52	0.45
1:F:150:GLY:O	1:F:151:LYS:C	2.59	0.45
1:D:257:ASN:N	1:D:257:ASN:OD1	2.50	0.45
1:F:230:VAL:O	1:F:234:ASP:HB2	2.18	0.45
1:D:41:PHE:O	1:D:42:GLU:C	2.59	0.44
1:B:96:ASP:HB3	1:B:100:TRP:CZ2	2.52	0.44
1:D:47:LYS:HA	1:D:272:LEU:HD12	2.00	0.44
1:E:54:PHE:HB3	1:E:55:PRO:HD2	1.99	0.44
1:B:22:ARG:HB3	1:B:23:PRO:HD3	1.98	0.44
1:F:103:GLN:HG3	1:F:133:ASN:O	2.18	0.44
1:C:8:MET:HE1	1:C:208:ILE:HD12	2.00	0.44
1:F:147:ASP:OD1	1:F:147:ASP:C	2.60	0.44
1:C:42:GLU:HB3	1:C:43:PRO:HD3	2.00	0.44
1:D:30:TYR:HA	1:D:34:ILE:HD12	1.99	0.44
1:A:107:ALA:N	4:A:2097:HOH:O	2.50	0.43
1:D:149:LYS:O	1:D:198:ARG:HA	2.17	0.43
1:C:12:ILE:HB	1:C:71:THR:HB	2.00	0.43
1:B:108:ALA:C	1:B:109:HIS:CG	2.96	0.43
1:E:153:ARG:NH2	1:E:160:ASN:OD1	2.51	0.43
1:B:150:GLY:O	1:B:151:LYS:C	2.60	0.43
1:C:180:LYS:O	1:C:184:GLU:HB2	2.19	0.43
1:A:22:ARG:O	1:A:23:PRO:C	2.60	0.43
1:D:22:ARG:HB3	1:D:23:PRO:HD3	2.00	0.42
1:D:249:PHE:CD1	1:D:250:PRO:HA	2.54	0.42
1:B:142:MET:HB2	1:B:143:TRP:CZ3	2.54	0.42
1:C:60:GLY:O	1:C:61:ASP:C	2.60	0.42
1:A:17:VAL:HB	4:A:2011:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:SER:HB3	1:B:41:PHE:CE2	2.55	0.42
1:F:2:ASP:HB2	4:F:2003:HOH:O	2.20	0.42
1:B:41:PHE:HD1	1:B:45:VAL:HB	1.85	0.41
1:D:182:LEU:HD23	1:D:183:PHE:CZ	2.55	0.41
1:F:149:LYS:HD2	1:F:191:GLN:HA	2.01	0.41
1:B:103:GLN:HA	1:B:133:ASN:O	2.21	0.41
1:B:109:HIS:HB3	4:B:2090:HOH:O	2.19	0.41
1:B:159:ALA:HB2	1:D:27:ARG:HD2	2.03	0.41
1:E:155:ILE:HD12	1:E:155:ILE:HA	1.92	0.41
1:B:187:VAL:O	1:B:188:PRO:C	2.62	0.41
1:F:103:GLN:HA	1:F:133:ASN:O	2.20	0.41
1:A:42:GLU:N	1:A:43:PRO:CD	2.84	0.41
1:C:47:LYS:HA	1:C:272:LEU:HD12	2.03	0.41
1:D:26:GLN:OE1	1:D:68:MET:HE1	2.21	0.41
1:E:140:LEU:HD21	1:E:216:VAL:CG2	2.51	0.41
1:C:249:PHE:CG	1:C:250:PRO:HA	2.56	0.41
1:D:168:GLY:O	1:D:257:ASN:HB3	2.21	0.40
1:C:155:ILE:HD12	1:C:155:ILE:HA	1.89	0.40
1:B:225:SER:OG	1:D:20:ASP:OD2	2.36	0.40
1:E:37:SER:HB3	1:E:41:PHE:CZ	2.56	0.40
1:C:229:LYS:O	1:C:233:ASP:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	256/282 (91%)	246 (96%)	10 (4%)	0	100	100
1	B	280/282 (99%)	267 (95%)	12 (4%)	1 (0%)	30	60
1	C	255/282 (90%)	246 (96%)	8 (3%)	1 (0%)	30	60
1	D	256/282 (91%)	250 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	255/282 (90%)	243 (95%)	12 (5%)	0	100	100
1	F	255/282 (90%)	245 (96%)	10 (4%)	0	100	100
All	All	1557/1692 (92%)	1497 (96%)	58 (4%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	ASP
1	C	207	ASP

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	225/240 (94%)	217 (96%)	8 (4%)	31	66
1	B	240/240 (100%)	239 (100%)	1 (0%)	84	94
1	C	226/240 (94%)	221 (98%)	5 (2%)	45	78
1	D	227/240 (95%)	224 (99%)	3 (1%)	61	86
1	E	226/240 (94%)	217 (96%)	9 (4%)	28	63
1	F	226/240 (94%)	218 (96%)	8 (4%)	32	67
All	All	1370/1440 (95%)	1336 (98%)	34 (2%)	43	76

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	4	LYS
1	A	85	GLU
1	A	87	LYS
1	A	103	GLN
1	A	131	GLU
1	A	151	LYS
1	A	185	LYS

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Mol	Chain	Res	Type
1	B	276	ARG
1	C	47	LYS
1	C	104	ILE
1	C	171	GLU
1	C	175	LYS
1	C	239	GLU
1	D	68	MET
1	D	91[A]	GLU
1	D	91[B]	GLU
1	E	71	THR
1	E	91	GLU
1	E	95	MET
1	E	103	GLN
1	E	104	ILE
1	E	131	GLU
1	E	185	LYS
1	E	197	THR
1	E	229	LYS
1	F	6	GLU
1	F	41	PHE
1	F	46	THR
1	F	91	GLU
1	F	103	GLN
1	F	151	LYS
1	F	239	GLU
1	F	240	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	B	109	HIS
1	B	257	ASN
1	C	26	GLN
1	C	101	GLN
1	C	103	GLN
1	C	274	ASN
1	D	101	GLN
1	D	103	GLN
1	E	101	GLN
1	E	224	GLN
1	E	257	ASN

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Mol	Chain	Res	Type
1	F	33	HIS
1	F	101	GLN
1	F	103	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](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
2	GOL	D	401	-	5,5,5	0.48	0	5,5,5	0.58	0
2	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.50	0
2	GOL	F	301	-	5,5,5	0.43	0	5,5,5	0.31	0
2	GOL	E	301	-	5,5,5	0.27	0	5,5,5	0.66	0
2	GOL	C	301	-	5,5,5	0.48	0	5,5,5	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	F	301	-	-	2/4/4/4	-
2	GOL	E	301	-	-	0/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	GOL	O1-C1-C2-C3
2	F	301	GOL	C1-C2-C3-O3
2	C	301	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-O2
2	F	301	GOL	O2-C2-C3-O3
2	C	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	260/282 (92%)	-0.08	3 (1%) 76 68	25, 32, 44, 61	0
1	B	282/282 (100%)	0.06	5 (1%) 67 58	29, 36, 57, 92	0
1	C	258/282 (91%)	-0.06	3 (1%) 76 68	20, 34, 49, 60	1 (0%)
1	D	258/282 (91%)	0.01	4 (1%) 70 61	19, 34, 50, 63	2 (0%)
1	E	258/282 (91%)	0.06	2 (0%) 82 75	21, 36, 51, 66	1 (0%)
1	F	258/282 (91%)	0.12	3 (1%) 76 68	21, 38, 54, 77	1 (0%)
All	All	1574/1692 (93%)	0.02	20 (1%) 75 66	19, 35, 53, 92	5 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	7.8
1	B	109	HIS	6.7
1	C	106	ALA	5.3
1	F	106	ALA	4.8
1	F	1	ALA	4.4
1	E	106	ALA	4.1
1	A	107	ALA	3.7
1	A	130	ALA	3.7
1	C	1	ALA	3.5
1	B	108	ALA	3.0
1	D	106	ALA	3.0
1	E	131	GLU	2.7
1	B	1	ALA	2.4
1	F	174	ASP	2.3
1	D	171	GLU	2.2
1	D	91[A]	GLU	2.2
1	D	207	ASP	2.1
1	B	115	ASP	2.1
1	B	239	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	207	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(Å ²)	Q<0.9
3	CL	C	401	1/1	0.76	0.12	42,42,42,42	0
3	CL	E	401	1/1	0.76	0.11	43,43,43,43	0
3	CL	B	401	1/1	0.79	0.10	50,50,50,50	0
2	GOL	E	301	6/6	0.85	0.15	45,49,50,51	0
2	GOL	D	401	6/6	0.86	0.16	40,48,50,51	0
3	CL	A	401	1/1	0.87	0.08	54,54,54,54	0
2	GOL	C	301	6/6	0.87	0.16	34,36,39,47	0
2	GOL	F	301	6/6	0.90	0.14	44,46,50,52	0
2	GOL	A	301	6/6	0.94	0.10	43,47,48,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.