



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID : 3QKE
Title : Crystal structure of D-mannonate dehydratase from Chromohalobacter Saalex-
 igens complexed with Mg and D-Gluconate
Authors : Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2011-02-01
Resolution : 1.55 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

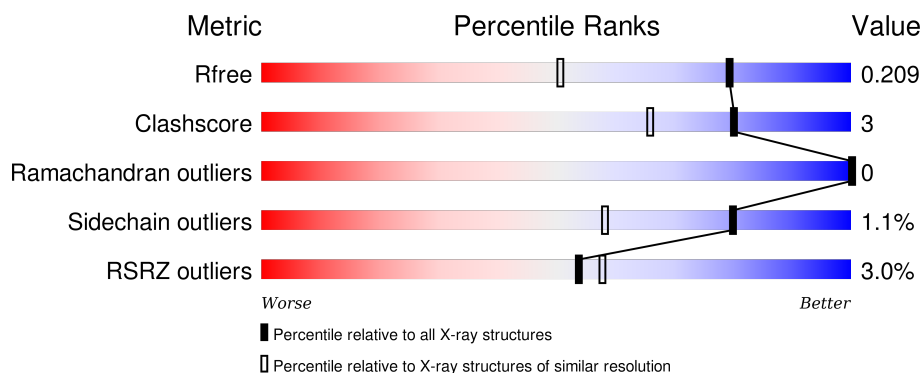
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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.



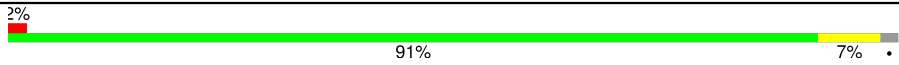
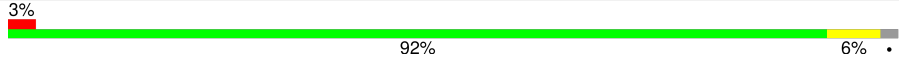
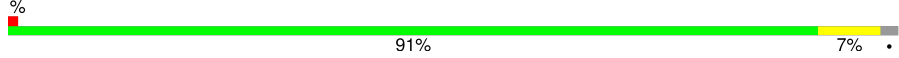
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	405	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	405	<div> <div>6%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	D	405	<div> <div>3%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	E	405	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	405	
1	G	405	
1	H	405	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GCO	A	406	-	-	-	X
2	GCO	H	406	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27932 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	397	Total	C	N	O	S	0	2	0
			3165	2005	566	580	14			
1	B	397	Total	C	N	O	S	0	2	0
			3165	2005	566	580	14			
1	C	397	Total	C	N	O	S	0	3	0
			3174	2010	567	583	14			
1	D	396	Total	C	N	O	S	0	3	0
			3169	2007	566	582	14			
1	E	397	Total	C	N	O	S	0	2	0
			3166	2005	566	581	14			
1	F	396	Total	C	N	O	S	0	2	0
			3160	2002	565	579	14			
1	G	397	Total	C	N	O	S	0	1	0
			3154	1999	562	579	14			
1	H	397	Total	C	N	O	S	0	1	0
			3154	1999	562	579	14			

There are 24 discrepancies between the modelled and reference sequences:

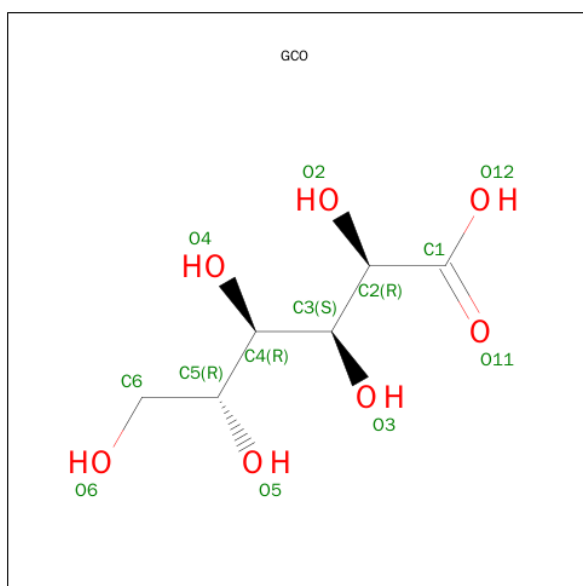
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q1QT89
A	2	SER	-	EXPRESSION TAG	UNP Q1QT89
A	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
B	1	MET	-	EXPRESSION TAG	UNP Q1QT89
B	2	SER	-	EXPRESSION TAG	UNP Q1QT89
B	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
C	1	MET	-	EXPRESSION TAG	UNP Q1QT89
C	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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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 SUGAR (GLUCONIC ACID) (three-letter code: GCO) (formula: C₆H₁₂O₇).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	302	Total	O	0	0
			302	302		
4	B	325	Total	O	0	0
			325	325		
4	C	264	Total	O	0	0
			264	264		
4	D	302	Total	O	0	0
			302	302		
4	E	308	Total	O	0	0
			308	308		
4	F	328	Total	O	0	0
			328	328		
4	G	337	Total	O	0	0
			337	337		

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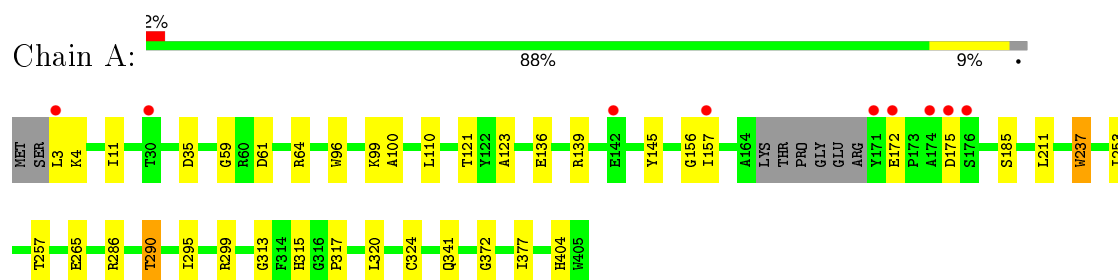
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	347	Total	O	0	0
			347	347		

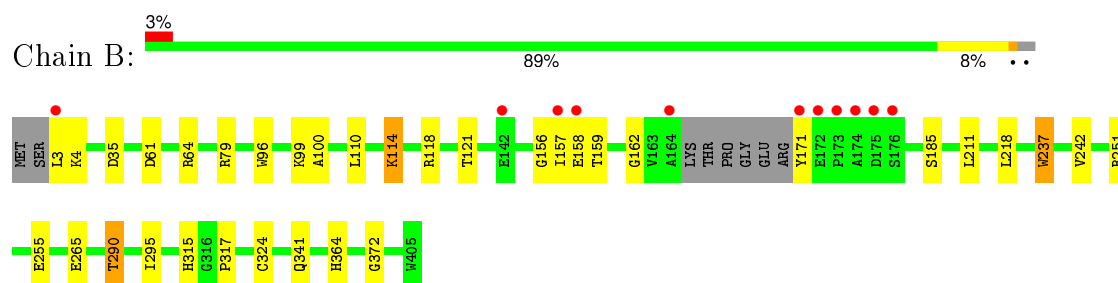
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

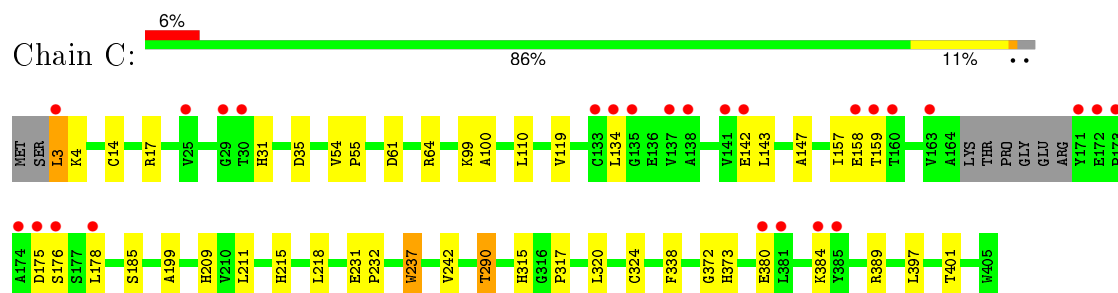
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



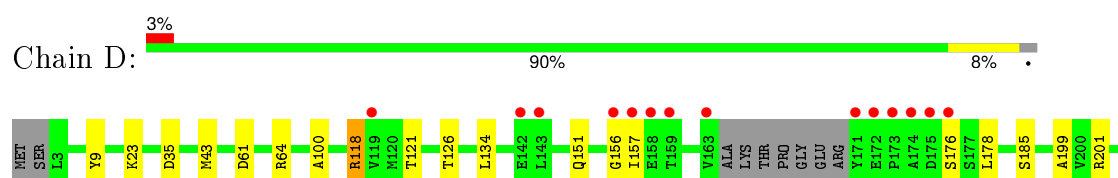
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

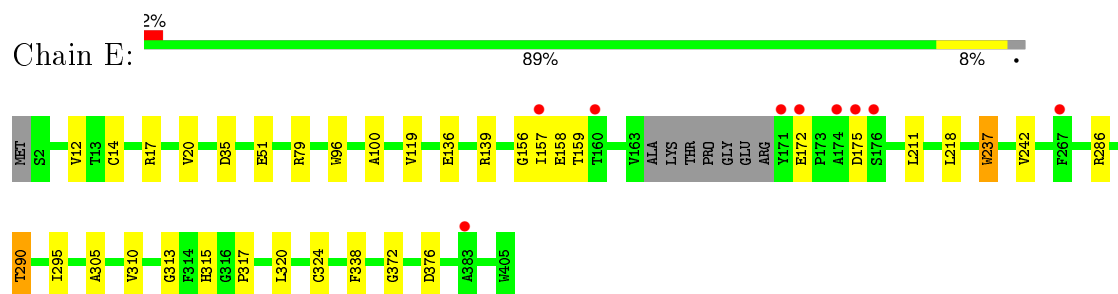


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

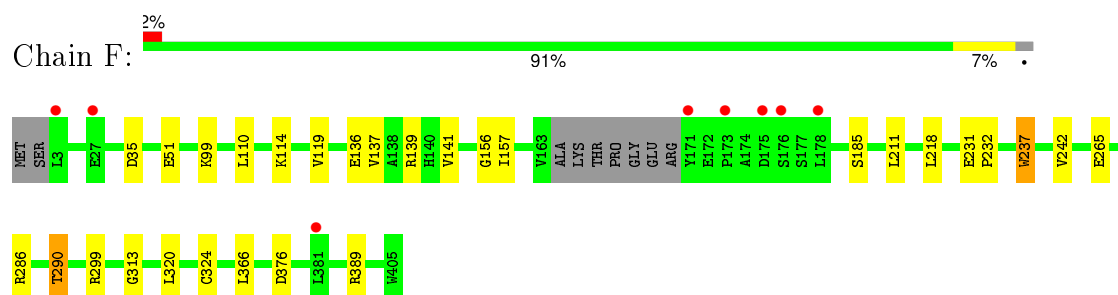




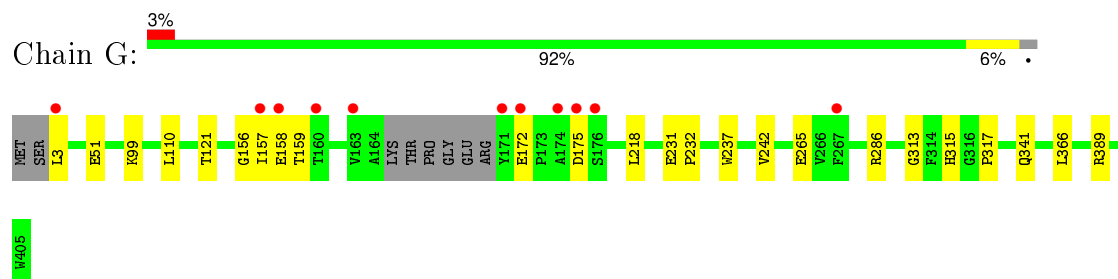
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



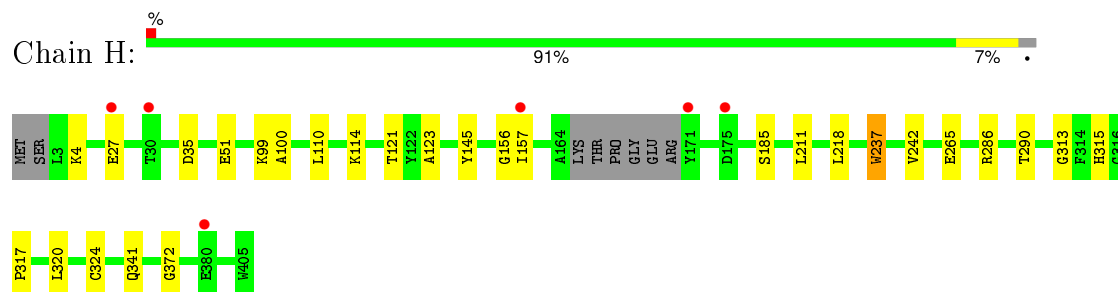
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.54Å 85.78Å 195.14Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	41.22 – 1.55 41.22 – 1.55	Depositor EDS
% Data completeness (in resolution range)	91.0 (41.22-1.55) 91.0 (41.22-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.179 , 0.211 0.178 , 0.209	Depositor DCC
R_{free} test set	20019 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 398167 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27932	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, GCO

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	0.34	0/3253	0.53	0/4430
1	B	0.34	0/3253	0.53	0/4430
1	C	0.33	0/3262	0.51	0/4442
1	D	0.33	0/3257	0.53	0/4435
1	E	0.31	0/3254	0.52	0/4431
1	F	0.34	0/3248	0.54	0/4423
1	G	0.34	0/3242	0.54	0/4416
1	H	0.34	0/3242	0.53	0/4416
All	All	0.33	0/26011	0.53	0/35423

There are no bond length outliers.

There are no bond angle outliers.

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	3165	0	3048	28	0
1	B	3165	0	3048	24	0
1	C	3174	0	3053	29	0
1	D	3169	0	3048	21	0
1	E	3166	0	3048	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3160	0	3043	21	0
1	G	3154	0	3036	12	0
1	H	3154	0	3036	22	0
2	A	13	0	10	1	0
2	B	13	0	10	1	0
2	C	13	0	11	0	0
2	D	13	0	10	0	0
2	E	13	0	10	0	0
2	F	13	0	10	1	0
2	G	13	0	10	1	0
2	H	13	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	302	0	0	0	0
4	B	325	0	0	0	0
4	C	264	0	0	3	0
4	D	302	0	0	0	0
4	E	308	0	0	1	0
4	F	328	0	0	0	0
4	G	337	0	0	0	0
4	H	347	0	0	0	0
All	All	27932	0	24442	167	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 3.

All (167) 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:380:GLU:HG2	4:C:1793:HOH:O	1.78	0.83
1:H:290:THR:HG23	1:H:324:CYS:SG	2.20	0.81
1:A:157:ILE:HD11	1:A:185:SER:HB3	1.66	0.77
1:F:290:THR:HG22	1:F:324:CYS:SG	2.25	0.77
1:E:290:THR:HG22	1:E:324:CYS:SG	2.26	0.76
1:C:290:THR:HG22	1:C:324:CYS:SG	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:ILE:HD11	1:H:185:SER:HB3	1.67	0.74
1:A:404:HIS:HD2	1:B:79:ARG:HH22	1.34	0.74
1:B:290:THR:HG22	1:B:324:CYS:SG	2.28	0.73
1:A:404:HIS:CD2	1:B:79:ARG:HH22	2.08	0.70
1:E:158:GLU:HG3	1:E:159:THR:HG23	1.75	0.68
1:F:136:GLU:OE2	1:F:139:ARG:HD3	1.95	0.67
1:B:156:GLY:O	1:B:157:ILE:HD13	1.96	0.66
1:A:290:THR:HG22	1:A:324:CYS:SG	2.35	0.66
1:H:4:LYS:HB3	1:H:27:GLU:HG3	1.78	0.66
1:B:158:GLU:HG3	1:B:159:THR:HG23	1.77	0.65
1:A:136:GLU:OE2	1:A:139:ARG:HD3	1.97	0.64
1:A:156:GLY:O	1:A:157:ILE:HD13	1.98	0.63
1:D:290:THR:HG22	1:D:324:CYS:SG	2.38	0.63
1:D:35:ASP:OD2	1:D:290:THR:HG21	1.99	0.62
1:E:136:GLU:OE2	1:E:139:ARG:HD3	2.00	0.62
1:D:218:LEU:O	1:D:242:VAL:HG12	1.99	0.62
1:E:100:ALA:HB3	1:E:372:GLY:HA2	1.83	0.61
1:B:61:ASP:HB3	1:B:64[A]:ARG:HG3	1.82	0.61
1:H:35:ASP:OD2	1:H:290:THR:HG21	2.01	0.60
1:G:156:GLY:O	1:G:157:ILE:HD13	2.00	0.60
1:C:142[B]:GLU:HG2	1:C:143:LEU:N	2.17	0.59
1:C:157:ILE:HD11	1:C:185:SER:HB3	1.83	0.59
1:H:156:GLY:O	1:H:157:ILE:HD13	2.02	0.59
1:A:35:ASP:OD2	1:A:290:THR:HG21	2.02	0.59
1:A:299:ARG:HD3	1:F:299:ARG:HD3	1.84	0.58
1:B:35:ASP:OD2	1:B:290:THR:HG21	2.03	0.58
1:B:290:THR:CG2	1:B:324:CYS:SG	2.92	0.57
1:D:156:GLY:O	1:D:157:ILE:HD13	2.03	0.57
1:A:100:ALA:HB3	1:A:372:GLY:HA2	1.87	0.56
1:C:3:LEU:HD12	1:C:4:LYS:N	2.20	0.56
1:B:99:LYS:HG3	1:B:110:LEU:HD21	1.88	0.56
1:C:315:HIS:CE1	1:C:317:PRO:HG3	2.41	0.56
1:C:290:THR:HG23	1:C:320:LEU:HD22	1.88	0.56
1:A:4:LYS:HE3	1:A:59:GLY:O	2.06	0.55
1:C:176:SER:HB2	1:C:178:LEU:O	2.06	0.55
1:A:172:GLU:O	1:A:175:ASP:HB2	2.07	0.55
1:F:286:ARG:HD2	1:F:313:GLY:O	2.06	0.55
1:E:35:ASP:OD2	1:E:290:THR:HG21	2.07	0.54
1:E:156:GLY:O	1:E:157:ILE:HD13	2.07	0.54
1:H:290:THR:OG1	1:H:320:LEU:HD22	2.08	0.54
1:H:35:ASP:HB3	1:H:290:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:LYS:HG2	1:G:110:LEU:HD21	1.90	0.53
1:C:3:LEU:HD12	1:C:4:LYS:H	1.72	0.53
1:C:290:THR:CG2	1:C:324:CYS:SG	2.96	0.53
1:F:35:ASP:OD2	1:F:290:THR:HG21	2.09	0.53
1:E:286:ARG:HD2	1:E:313:GLY:O	2.08	0.53
1:F:290:THR:HG23	1:F:320:LEU:HD22	1.91	0.53
1:E:315:HIS:CE1	1:E:317:PRO:HG3	2.44	0.53
1:A:64[B]:ARG:CZ	1:F:114:LYS:HD2	2.39	0.53
1:C:35:ASP:OD2	1:C:290:THR:HG21	2.09	0.52
1:E:290:THR:HG23	1:E:320:LEU:HD22	1.91	0.52
1:F:157:ILE:HD11	1:F:185:SER:HB3	1.90	0.52
1:H:100:ALA:HB3	1:H:372:GLY:HA2	1.92	0.52
1:C:389:ARG:HD3	1:E:51:GLU:OE2	2.10	0.52
1:A:290:THR:CG2	1:A:324:CYS:SG	2.98	0.51
1:B:118:ARG:HD2	1:B:364:HIS:CG	2.46	0.51
1:H:123:ALA:HB2	1:H:145:TYR:CE2	2.46	0.51
1:F:156:GLY:O	1:F:157:ILE:HD13	2.11	0.51
1:E:119:VAL:HG13	1:E:338:PHE:CZ	2.46	0.50
1:D:43:MET:HG3	1:H:51:GLU:HG2	1.93	0.50
1:E:79:ARG:HA	4:E:984:HOH:O	2.11	0.50
1:D:286:ARG:HD2	1:D:313:GLY:O	2.12	0.50
1:D:176:SER:HB2	1:D:178:LEU:O	2.12	0.49
1:F:211:LEU:HD23	1:F:237:TRP:CE2	2.46	0.49
1:D:43:MET:CG	1:H:51:GLU:HG2	2.43	0.49
1:D:290:THR:CG2	1:D:324:CYS:SG	3.01	0.49
1:H:286:ARG:HD2	1:H:313:GLY:O	2.13	0.49
1:C:61:ASP:HB3	1:C:64[A]:ARG:HG3	1.94	0.49
1:C:31:HIS:CE1	4:C:2528:HOH:O	2.65	0.49
1:F:51:GLU:OE2	1:G:389:ARG:HD3	2.13	0.49
1:G:218:LEU:O	1:G:242:VAL:HG12	2.12	0.48
1:B:162:GLY:HA2	1:B:171:TYR:CE2	2.48	0.48
1:E:211:LEU:HD23	1:E:237:TRP:CE2	2.48	0.48
1:C:290:THR:CG2	1:C:320:LEU:HD22	2.43	0.48
1:A:315:HIS:CE1	1:A:317:PRO:HG3	2.48	0.48
1:A:286:ARG:HD2	1:A:313:GLY:O	2.13	0.48
1:A:136:GLU:HA	1:A:139:ARG:HG2	1.96	0.48
1:E:305:ALA:HB1	1:E:310:VAL:HB	1.95	0.48
1:B:118:ARG:HD2	1:B:364:HIS:CD2	2.48	0.47
1:B:157:ILE:HD11	1:B:185:SER:HB3	1.95	0.47
1:H:265:GLU:OE2	2:H:406:GCO:H2	2.15	0.47
1:C:100:ALA:HB3	1:C:372:GLY:HA2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:LEU:O	1:H:242:VAL:HG12	2.15	0.47
1:C:14:CYS:HA	1:C:17:ARG:O	2.15	0.47
1:D:157:ILE:HD11	1:D:185:SER:CB	2.45	0.47
1:H:290:THR:CG2	1:H:324:CYS:HB2	2.45	0.46
1:C:211:LEU:HD23	1:C:237:TRP:CE2	2.51	0.46
1:F:136:GLU:HA	1:F:139:ARG:HG2	1.97	0.45
1:C:119:VAL:HG13	1:C:338:PHE:CZ	2.51	0.45
1:A:265:GLU:OE2	2:A:406:GCO:H2	2.15	0.45
1:C:134:LEU:HD11	1:C:199:ALA:HB1	1.99	0.45
1:C:384:LYS:HE2	4:C:2544:HOH:O	2.16	0.45
1:H:123:ALA:HB2	1:H:145:TYR:CD2	2.52	0.45
1:E:290:THR:CG2	1:E:324:CYS:SG	3.00	0.45
1:E:14:CYS:HA	1:E:17:ARG:O	2.17	0.45
1:F:366:LEU:HD22	1:F:366:LEU:N	2.32	0.45
1:H:211:LEU:HD23	1:H:237:TRP:CE2	2.52	0.45
1:C:64[B]:ARG:CZ	1:H:114:LYS:HE3	2.47	0.44
1:C:397:LEU:HD12	1:C:401:THR:HB	1.99	0.44
1:A:64[B]:ARG:NH2	1:F:114:LYS:HD2	2.32	0.44
1:G:121:THR:HA	1:G:341:GLN:O	2.16	0.44
1:F:389:ARG:HD3	1:G:51:GLU:OE2	2.17	0.44
1:C:158:GLU:HG3	1:C:159:THR:HG23	1.99	0.44
1:B:100:ALA:HB3	1:B:372:GLY:HA2	1.99	0.44
1:A:290:THR:HG23	1:A:320:LEU:HD22	1.99	0.44
1:C:99:LYS:HG2	1:C:110:LEU:HD21	1.98	0.44
1:F:265:GLU:OE2	2:F:406:GCO:H2	2.17	0.44
1:D:9:TYR:CZ	1:D:23:LYS:HD3	2.53	0.44
1:F:218:LEU:O	1:F:242:VAL:HG12	2.18	0.44
1:H:99:LYS:HG2	1:H:110:LEU:HD21	2.00	0.44
1:D:118:ARG:HD2	1:D:364:HIS:ND1	2.32	0.44
1:D:61:ASP:HB3	1:D:64[A]:ARG:HG3	1.99	0.43
1:B:121:THR:HA	1:B:341:GLN:O	2.18	0.43
1:B:114:LYS:HB2	1:B:114:LYS:HE3	1.62	0.43
1:B:290:THR:CG2	1:B:324:CYS:HB2	2.49	0.43
1:E:12:VAL:HG22	1:E:20:VAL:HG22	2.00	0.43
1:F:99:LYS:HG2	1:F:110:LEU:HD21	2.00	0.43
1:E:218:LEU:O	1:E:242:VAL:HG12	2.18	0.43
1:F:290:THR:CG2	1:F:320:LEU:HD22	2.49	0.43
1:C:218:LEU:O	1:C:242:VAL:HG12	2.18	0.43
1:A:99:LYS:HG2	1:A:110:LEU:HD21	2.00	0.43
1:E:96:TRP:CD1	1:E:295:ILE:HB	2.53	0.43
1:D:134:LEU:HD11	1:D:199:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:CG2	1:A:324:CYS:HB2	2.49	0.42
1:D:157:ILE:HD11	1:D:185:SER:HB3	2.00	0.42
1:D:118:ARG:HD2	1:D:364:HIS:CE1	2.54	0.42
1:H:315:HIS:CE1	1:H:317:PRO:HG3	2.55	0.42
1:B:315:HIS:CE1	1:B:317:PRO:HG3	2.55	0.42
1:A:253:ILE:O	1:A:257:THR:HG22	2.20	0.42
1:H:157:ILE:HD11	1:H:185:SER:CB	2.44	0.42
1:B:3:LEU:CD2	1:B:4:LYS:HE3	2.50	0.42
1:D:121:THR:HA	1:D:341:GLN:O	2.19	0.42
1:G:265:GLU:OE2	2:G:406:GCO:H2	2.19	0.42
1:A:211:LEU:HD23	1:A:237:TRP:CE2	2.55	0.42
1:B:251[A]:ARG:O	1:B:255:GLU:HG3	2.19	0.42
1:B:218:LEU:O	1:B:242:VAL:HG12	2.19	0.41
1:B:265:GLU:OE2	2:B:406:GCO:H2	2.19	0.41
1:G:158:GLU:HG3	1:G:159:THR:HG23	2.01	0.41
1:A:61:ASP:HB3	1:A:64[A]:ARG:HG3	2.02	0.41
1:E:172:GLU:O	1:E:175:ASP:HB2	2.20	0.41
1:D:343:HIS:CD2	1:D:365:PHE:HZ	2.39	0.41
1:G:231:GLU:N	1:G:232:PRO:CD	2.84	0.41
1:A:123:ALA:HB2	1:A:145:TYR:CE2	2.56	0.41
1:D:126:THR:HA	1:D:151:GLN:O	2.20	0.41
1:G:366:LEU:HD22	1:G:366:LEU:N	2.36	0.41
1:G:286:ARG:HD2	1:G:313:GLY:O	2.20	0.41
1:D:100:ALA:HB3	1:D:372:GLY:HA2	2.02	0.41
1:H:121:THR:HA	1:H:341:GLN:O	2.20	0.41
1:B:211:LEU:HD23	1:B:237:TRP:CE2	2.56	0.41
1:C:231:GLU:N	1:C:232:PRO:CD	2.83	0.41
1:F:137:VAL:O	1:F:141:VAL:HG23	2.20	0.41
1:C:54:VAL:HB	1:C:55:PRO:HD3	2.03	0.41
1:F:231:GLU:N	1:F:232:PRO:CD	2.83	0.41
1:A:96:TRP:CD1	1:A:295:ILE:HB	2.56	0.41
1:E:211:LEU:HD12	1:E:211:LEU:N	2.37	0.40
1:G:315:HIS:CE1	1:G:317:PRO:HG3	2.56	0.40
1:B:96:TRP:CD1	1:B:295:ILE:HB	2.56	0.40
1:A:121:THR:HA	1:A:341:GLN:O	2.21	0.40
1:A:11:ILE:HD13	1:A:377:ILE:HD13	2.04	0.40
1:C:147:ALA:CB	1:C:209:HIS:HB2	2.51	0.40
1:D:201:ARG:HD3	1:D:201:ARG:HA	1.90	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	395/405 (98%)	384 (97%)	11 (3%)	0	100	100
1	B	395/405 (98%)	385 (98%)	10 (2%)	0	100	100
1	C	396/405 (98%)	384 (97%)	12 (3%)	0	100	100
1	D	395/405 (98%)	383 (97%)	12 (3%)	0	100	100
1	E	395/405 (98%)	384 (97%)	11 (3%)	0	100	100
1	F	394/405 (97%)	381 (97%)	13 (3%)	0	100	100
1	G	394/405 (97%)	382 (97%)	12 (3%)	0	100	100
1	H	394/405 (97%)	382 (97%)	12 (3%)	0	100	100
All	All	3158/3240 (98%)	3065 (97%)	93 (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	327/332 (98%)	324 (99%)	3 (1%)	84	66
1	B	327/332 (98%)	324 (99%)	3 (1%)	84	66
1	C	328/332 (99%)	322 (98%)	6 (2%)	66	36
1	D	328/332 (99%)	323 (98%)	5 (2%)	72	44
1	E	328/332 (99%)	325 (99%)	3 (1%)	84	66
1	F	327/332 (98%)	323 (99%)	4 (1%)	78	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	326/332 (98%)	322 (99%)	4 (1%)	78	54
1	H	326/332 (98%)	325 (100%)	1 (0%)	94	86
All	All	2617/2656 (98%)	2588 (99%)	29 (1%)	80	58

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	237	TRP
1	A	290	THR
1	B	114	LYS
1	B	237	TRP
1	B	290	THR
1	C	3	LEU
1	C	175	ASP
1	C	215	HIS
1	C	237	TRP
1	C	290	THR
1	C	373	HIS
1	D	118	ARG
1	D	215	HIS
1	D	237	TRP
1	D	290	THR
1	D	366	LEU
1	E	237	TRP
1	E	290	THR
1	E	376	ASP
1	F	119	VAL
1	F	237	TRP
1	F	290	THR
1	F	376	ASP
1	G	3	LEU
1	G	172	GLU
1	G	175	ASP
1	G	237	TRP
1	H	237	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	278	GLN
1	A	404	HIS
1	B	128	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 carbohydrates 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	$\# Z > 2$
2	GCO	A	406	3	8,12,12	0.44	0	10,16,16	1.54	1 (10%)
2	GCO	B	406	3	8,12,12	0.35	0	10,16,16	1.33	1 (10%)
2	GCO	C	406	3	8,12,12	0.41	0	10,16,16	1.44	1 (10%)
2	GCO	D	406	3	8,12,12	0.41	0	10,16,16	1.36	2 (20%)
2	GCO	E	406	3	8,12,12	0.38	0	10,16,16	1.27	1 (10%)
2	GCO	F	406	3	8,12,12	0.34	0	10,16,16	1.22	1 (10%)
2	GCO	G	406	3	8,12,12	0.28	0	10,16,16	1.44	2 (20%)
2	GCO	H	406	3	8,12,12	0.38	0	10,16,16	1.74	1 (10%)

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	GCO	A	406	3	-	0/14/18/18	0/0/0/0
2	GCO	B	406	3	-	0/14/18/18	0/0/0/0
2	GCO	C	406	3	-	0/14/18/18	0/0/0/0
2	GCO	D	406	3	-	0/14/18/18	0/0/0/0
2	GCO	E	406	3	-	0/14/18/18	0/0/0/0
2	GCO	F	406	3	-	0/14/18/18	0/0/0/0
2	GCO	G	406	3	-	0/14/18/18	0/0/0/0
2	GCO	H	406	3	-	0/14/18/18	0/0/0/0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	406	GCO	C4-C3-C2	-4.59	105.58	113.63
2	A	406	GCO	C4-C3-C2	-3.79	106.98	113.63
2	C	406	GCO	C4-C3-C2	-3.61	107.30	113.63
2	G	406	GCO	C4-C3-C2	-3.41	107.64	113.63
2	B	406	GCO	C4-C3-C2	-3.30	107.83	113.63
2	E	406	GCO	C4-C3-C2	-3.21	108.00	113.63
2	D	406	GCO	C5-C4-C3	-3.12	107.39	112.47
2	F	406	GCO	C4-C3-C2	-2.67	108.94	113.63
2	D	406	GCO	C4-C3-C2	-2.33	109.53	113.63
2	G	406	GCO	C5-C4-C3	-2.14	108.98	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	406	GCO	1	0
2	B	406	GCO	1	0
2	F	406	GCO	1	0
2	G	406	GCO	1	0
2	H	406	GCO	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	397/405 (98%)	-0.24	9 (2%) 64 67	17, 22, 36, 55	0
1	B	397/405 (98%)	-0.17	11 (2%) 56 60	17, 22, 35, 57	0
1	C	397/405 (98%)	0.18	26 (6%) 22 22	19, 25, 39, 60	0
1	D	396/405 (97%)	0.00	14 (3%) 48 51	19, 25, 40, 58	0
1	E	397/405 (98%)	-0.09	9 (2%) 64 67	17, 25, 38, 53	0
1	F	396/405 (97%)	-0.14	8 (2%) 68 71	17, 22, 36, 48	0
1	G	397/405 (98%)	-0.27	11 (2%) 56 60	17, 21, 34, 59	0
1	H	397/405 (98%)	-0.30	6 (1%) 76 79	17, 22, 33, 44	0
All	All	3174/3240 (97%)	-0.13	94 (2%) 54 58	17, 23, 37, 60	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	TYR	9.8
1	D	171	TYR	7.2
1	D	175	ASP	7.2
1	B	171	TYR	7.2
1	C	175	ASP	6.7
1	E	175	ASP	6.6
1	B	175	ASP	6.3
1	F	171	TYR	5.9
1	A	175	ASP	5.5
1	G	175	ASP	5.2
1	G	171	TYR	5.0
1	E	171	TYR	4.8
1	C	138	ALA	4.7
1	G	174	ALA	4.4
1	A	171	TYR	4.4
1	C	141	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	176	SER	4.2
1	C	172	GLU	4.2
1	D	176	SER	4.2
1	E	176	SER	4.2
1	B	174	ALA	4.0
1	F	3	LEU	3.8
1	A	174	ALA	3.7
1	E	174	ALA	3.6
1	A	3	LEU	3.6
1	G	157	ILE	3.5
1	B	173	PRO	3.5
1	A	176	SER	3.4
1	D	173	PRO	3.4
1	C	174	ALA	3.4
1	F	175	ASP	3.4
1	D	172	GLU	3.4
1	C	3	LEU	3.3
1	C	158	GLU	3.3
1	D	143	LEU	3.2
1	B	3	LEU	3.2
1	G	158	GLU	3.1
1	B	172	GLU	3.0
1	D	158	GLU	3.0
1	D	174	ALA	3.0
1	C	159	THR	3.0
1	C	133	CYS	3.0
1	G	172	GLU	3.0
1	C	176	SER	2.9
1	C	25	VAL	2.9
1	C	380	GLU	2.8
1	C	384	LYS	2.8
1	C	173	PRO	2.8
1	B	164	ALA	2.8
1	C	142[A]	GLU	2.8
1	F	27	GLU	2.8
1	F	173	PRO	2.7
1	C	134	LEU	2.7
1	D	119	VAL	2.7
1	G	163	VAL	2.7
1	D	159	THR	2.7
1	D	156	GLY	2.7
1	H	175	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	163	VAL	2.7
1	G	3	LEU	2.7
1	B	157	ILE	2.6
1	D	157	ILE	2.6
1	C	160	THR	2.6
1	E	383	ALA	2.5
1	A	142	GLU	2.5
1	C	178	LEU	2.5
1	C	163	VAL	2.5
1	D	142	GLU	2.5
1	F	176	SER	2.5
1	H	380	GLU	2.5
1	E	157	ILE	2.5
1	H	157	ILE	2.4
1	G	176	SER	2.4
1	G	160	THR	2.4
1	H	171	TYR	2.3
1	F	381	LEU	2.3
1	B	158	GLU	2.3
1	C	385	TYR	2.2
1	C	30	THR	2.2
1	E	172	GLU	2.1
1	A	157	ILE	2.1
1	E	267	PHE	2.1
1	C	137	VAL	2.1
1	H	27	GLU	2.1
1	C	29	GLY	2.1
1	C	135	GLY	2.1
1	C	381	LEU	2.1
1	F	178	LEU	2.1
1	B	142	GLU	2.1
1	A	172	GLU	2.0
1	G	267	PHE	2.0
1	H	30	THR	2.0
1	A	30	THR	2.0
1	E	160	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GCO	H	406	13/13	0.87	0.13	3.25	22,30,35,38	0
2	GCO	A	406	13/13	0.88	0.13	2.76	22,30,35,40	0
2	GCO	G	406	13/13	0.89	0.12	1.76	22,27,34,35	0
2	GCO	E	406	13/13	0.86	0.13	1.76	23,32,36,39	0
3	MG	B	407	1/1	1.00	0.10	1.40	21,21,21,21	0
3	MG	A	407	1/1	1.00	0.10	1.21	21,21,21,21	0
3	MG	G	407	1/1	0.99	0.10	1.10	21,21,21,21	0
3	MG	F	407	1/1	0.99	0.09	0.75	21,21,21,21	0
2	GCO	C	406	13/13	0.83	0.16	0.71	26,33,41,43	0
2	GCO	F	406	13/13	0.87	0.12	0.58	21,30,35,40	0
2	GCO	B	406	13/13	0.91	0.11	0.45	22,29,35,38	0
2	GCO	D	406	13/13	0.84	0.12	0.43	23,31,36,42	0
3	MG	H	407	1/1	1.00	0.08	0.08	19,19,19,19	0
3	MG	E	407	1/1	1.00	0.08	-0.25	22,22,22,22	0
3	MG	D	407	1/1	0.99	0.08	-0.44	24,24,24,24	0
3	MG	C	407	1/1	0.98	0.07	-0.75	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.