



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:00 AM GMT

PDB ID : 2OZR
Title : MMP13 Catalytic Domain Complexed with 4-{{[1-methyl-2,4-dioxo-6-(3-phenylprop-1-yn-1-yl)-1,4-dihydroquinazolin-3(2H)-yl]methyl}benzoic acid
Authors : Johnson, A.R.; Pavlovsky, A.G.; Ortwine, D.F.; Prior, F.; Man, C.-F.; Bornemeier, D.A.; Banotai, C.A.; Mueller, W.T.; McConnell, P.; Yan, C.H.; Baragi, V.; Lesch, C.; Roark, W.H.; Lie, J.J.; Fasquelle, V.; Wilson, M.; Robertson, D.; Datta, K.; Guzman, R.; Han, H.-K.; Dyer, R.D.
Deposited on : 2007-02-27
Resolution : 2.30 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

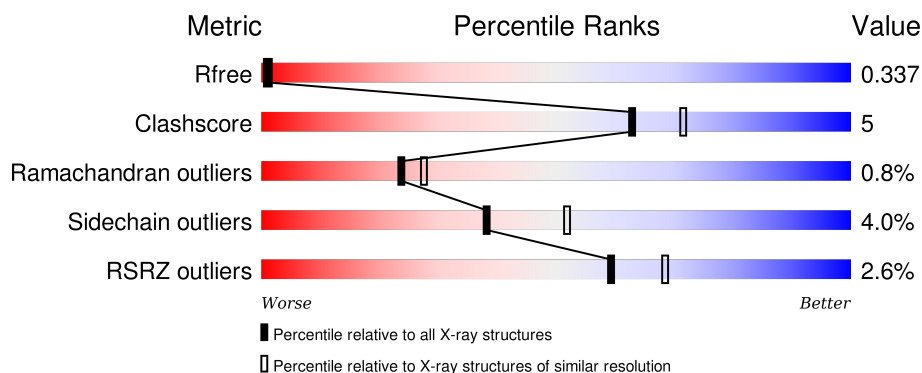
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	170	<div> <div>92%</div> <div>6%</div> </div>
1	B	170	<div> <div>88%</div> <div>9%</div> </div>
1	C	170	<div> <div>3%</div> <div>87%</div> <div>11%</div> </div>
1	D	170	<div> <div>88%</div> <div>9%</div> </div>
1	E	170	<div> <div>4%</div> <div>80%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	170	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	G	170	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>...</div> </div> </div>
1	H	170	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>

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
5	HAE	C	3001	-	-	-	X
5	HAE	D	3002	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11898 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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	7	0
			1329	861	215	248	5			
1	B	167	Total	C	N	O	S	0	7	0
			1329	861	215	248	5			
1	C	167	Total	C	N	O	S	0	7	0
			1330	861	215	249	5			
1	D	166	Total	C	N	O	S	0	7	0
			1318	852	214	247	5			
1	E	164	Total	C	N	O	S	0	7	0
			1305	846	209	245	5			
1	F	167	Total	C	N	O	S	0	6	0
			1330	861	215	249	5			
1	G	166	Total	C	N	O	S	0	7	0
			1321	857	214	245	5			
1	H	163	Total	C	N	O	S	0	6	0
			1296	842	208	241	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	MET	-	EXPRESSION TAG	UNP P45452
A	81	ALA	-	EXPRESSION TAG	UNP P45452
A	82	SER	-	EXPRESSION TAG	UNP P45452
B	80	MET	-	EXPRESSION TAG	UNP P45452
B	81	ALA	-	EXPRESSION TAG	UNP P45452
B	82	SER	-	EXPRESSION TAG	UNP P45452
C	80	MET	-	EXPRESSION TAG	UNP P45452
C	81	ALA	-	EXPRESSION TAG	UNP P45452
C	82	SER	-	EXPRESSION TAG	UNP P45452
D	80	MET	-	EXPRESSION TAG	UNP P45452
D	81	ALA	-	EXPRESSION TAG	UNP P45452
D	82	SER	-	EXPRESSION TAG	UNP P45452
E	80	MET	-	EXPRESSION TAG	UNP P45452

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Chain	Residue	Modelled	Actual	Comment	Reference
E	81	ALA	-	EXPRESSION TAG	UNP P45452
E	82	SER	-	EXPRESSION TAG	UNP P45452
F	80	MET	-	EXPRESSION TAG	UNP P45452
F	81	ALA	-	EXPRESSION TAG	UNP P45452
F	82	SER	-	EXPRESSION TAG	UNP P45452
G	80	MET	-	EXPRESSION TAG	UNP P45452
G	81	ALA	-	EXPRESSION TAG	UNP P45452
G	82	SER	-	EXPRESSION TAG	UNP P45452
H	80	MET	-	EXPRESSION TAG	UNP P45452
H	81	ALA	-	EXPRESSION TAG	UNP P45452
H	82	SER	-	EXPRESSION TAG	UNP P45452

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

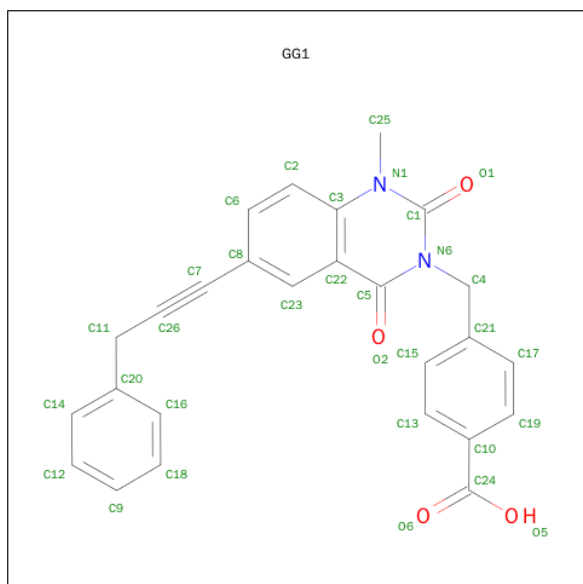
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Ca 3 3	0	0
3	D	3	Total Ca 3 3	0	0
3	E	3	Total Ca 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0
3	A	3	Total 3	Ca 3	0	0
3	F	3	Total 3	Ca 3	0	0

- Molecule 4 is 4-{[1-METHYL-2,4-DIOXO-6-(3-PHENYLPROP-1-YN-1-YL)-1,4-DIHYDROQUINAZOLIN-3(2H)-YL]METHYL}BENZOIC ACID (three-letter code: GG1) (formula: C₂₆H₂₀N₂O₄).



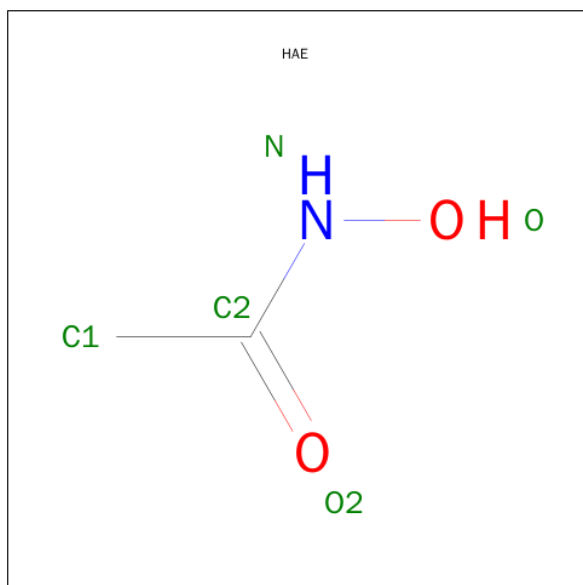
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 32	C 26	N 2	O 4	0	0
4	B	1	Total 32	C 26	N 2	O 4	0	0
4	C	1	Total 32	C 26	N 2	O 4	0	0
4	D	1	Total 32	C 26	N 2	O 4	0	0
4	E	1	Total 32	C 26	N 2	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			32	26	2	4		
4	G	1	Total	C	N	O	0	0
			32	26	2	4		
4	H	1	Total	C	N	O	0	0
			32	26	2	4		

- Molecule 5 is ACETOHYDROXAMIC ACID (three-letter code: HAE) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		
5	E	1	Total	C	N	O	0	0
			5	2	1	2		
5	F	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total	O	0	0
			134	134		
6	B	128	Total	O	0	0
			128	128		

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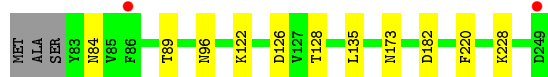
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	150	Total 150	O 150	0	0
6	D	141	Total 141	O 141	0	0
6	E	114	Total 114	O 114	0	0
6	F	115	Total 115	O 115	0	0
6	G	126	Total 126	O 126	0	0
6	H	116	Total 116	O 116	0	0

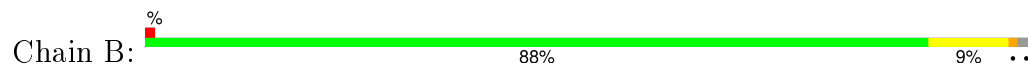
3 Residue-property plots [i](#)

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.

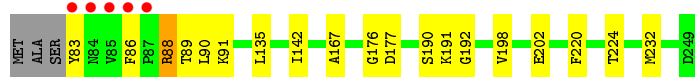
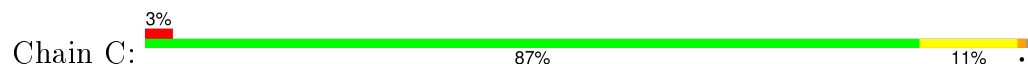
• Molecule 1: Collagenase 3



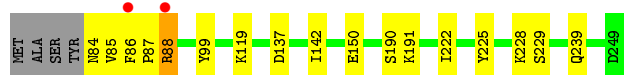
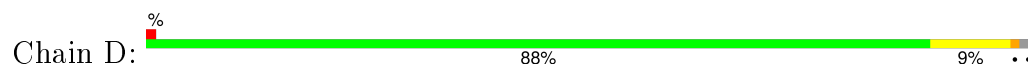
• Molecule 1: Collagenase 3



• Molecule 1: Collagenase 3



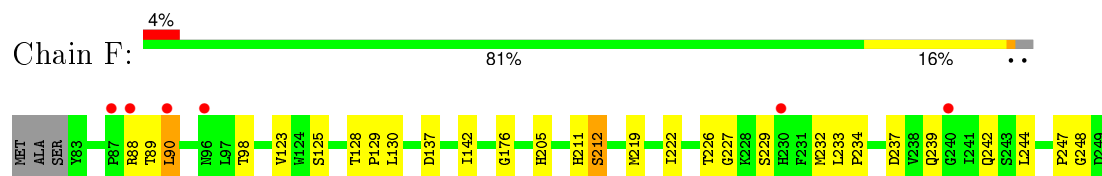
• Molecule 1: Collagenase 3



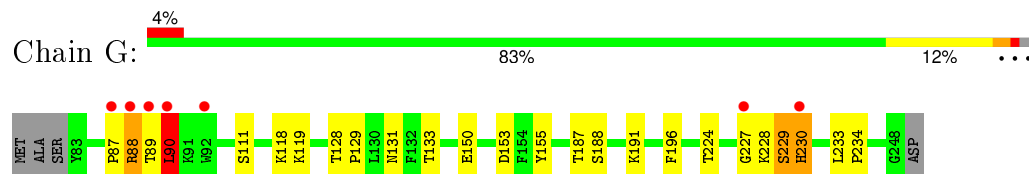
• Molecule 1: Collagenase 3



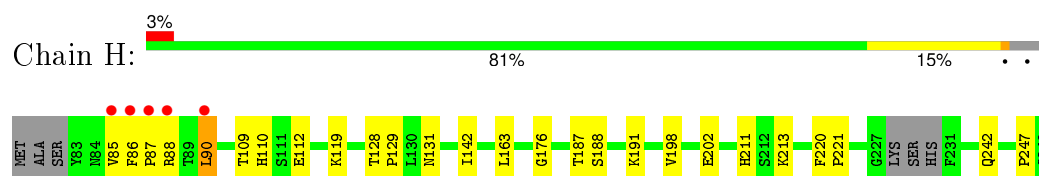
• Molecule 1: Collagenase 3



- Molecule 1: Collagenase 3



- Molecule 1: Collagenase 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.84Å 71.97Å 138.13Å 90.00° 124.59° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.46 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-2.30) 90.3 (49.46-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.340 0.246 , 0.337	Depositor DCC
R_{free} test set	2869 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 71.7	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	5 of 69624 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11898	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 93.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.8535e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, GG1, CA, HAE

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	0.49	0/1377	0.57	0/1872
1	B	0.48	0/1377	0.57	0/1872
1	C	0.47	0/1378	0.57	0/1872
1	D	0.49	0/1365	0.61	0/1854
1	E	0.48	0/1351	0.57	0/1835
1	F	0.48	0/1378	0.62	0/1872
1	G	0.46	0/1369	0.58	0/1861
1	H	0.45	0/1342	0.57	0/1824
All	All	0.48	0/10937	0.58	0/14862

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	1329	0	1226	6	1
1	B	1329	0	1226	14	0
1	C	1330	0	1226	14	0
1	D	1318	0	1217	16	0
1	E	1305	0	1200	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1330	0	1228	21	0
1	G	1321	0	1222	26	0
1	H	1296	0	1198	14	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	32	0	19	1	0
4	B	32	0	19	1	0
4	C	32	0	19	1	0
4	D	32	0	19	1	0
4	E	32	0	19	0	0
4	F	32	0	19	1	0
4	G	32	0	19	0	0
4	H	32	0	19	1	0
5	C	5	0	4	1	0
5	D	5	0	5	0	0
5	E	5	0	5	0	0
5	F	5	0	4	0	0
6	A	134	0	0	2	0
6	B	128	0	0	1	0
6	C	150	0	0	1	0
6	D	141	0	0	2	0
6	E	114	0	0	0	0
6	F	115	0	0	0	0
6	G	126	0	0	1	0
6	H	116	0	0	2	0
All	All	11898	0	9913	110	1

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 5.

All (110) 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:G:88:ARG:HA	1:G:89:THR:HB	1.25	1.17
1:G:227:GLY:HA3	1:G:228:LYS:HB3	1.32	1.07
1:D:85:VAL:HG11	1:F:244:LEU:HD21	1.40	1.00
1:G:88:ARG:HH11	1:G:88:ARG:HB3	1.29	0.97
1:B:100:ARG:HB3	1:B:143:MET:CE	1.96	0.96
1:B:100:ARG:HB3	1:B:143:MET:HE1	1.51	0.92
1:H:119:LYS:HE3	6:H:4143:HOH:O	1.75	0.85
1:D:85:VAL:CG1	1:F:244:LEU:HD21	2.06	0.85
1:G:88:ARG:HA	1:G:89:THR:CB	2.02	0.84
1:G:227:GLY:HA3	1:G:228:LYS:CB	2.07	0.84
1:G:88:ARG:HB3	1:G:88:ARG:NH1	2.00	0.76
1:H:88:ARG:HB3	1:H:90:LEU:HG	1.68	0.76
1:F:226:THR:HB	1:F:227:GLY:HA3	1.69	0.75
1:A:128:THR:O	6:A:4106:HOH:O	2.10	0.70
1:D:85:VAL:HG11	1:F:244:LEU:CD2	2.20	0.70
1:B:88:ARG:H	1:B:88:ARG:HD3	1.58	0.68
1:H:86:PHE:HB2	6:H:4147:HOH:O	1.95	0.66
1:B:100:ARG:HB3	1:B:143:MET:HE2	1.76	0.65
1:G:87:PRO:O	1:G:88:ARG:NH1	2.30	0.65
1:G:88:ARG:HG2	1:G:89:THR:C	2.18	0.63
1:B:88:ARG:CD	1:B:88:ARG:H	2.12	0.63
1:A:89:THR:HG22	6:A:4116:HOH:O	1.98	0.63
1:G:119:LYS:HG2	1:G:196:PHE:CE2	2.34	0.62
1:C:83:TYR:HB2	1:E:240:GLY:CA	2.29	0.62
1:E:239:GLN:HG2	1:G:230:HIS:HB2	1.82	0.62
1:C:83:TYR:HB2	1:E:240:GLY:HA2	1.83	0.60
1:E:242:GLN:NE2	1:E:247:PRO:HA	2.19	0.58
1:B:143:MET:HA	1:B:143:MET:CE	2.34	0.57
1:A:135:LEU:HD21	1:B:222:ILE:HG12	1.87	0.55
1:A:122:LYS:NZ	1:A:126:ASP:OD1	2.40	0.55
1:A:220:PHE:O	4:A:2001:GG1:H16	2.07	0.55
1:F:128:THR:HB	1:F:129:PRO:HD2	1.89	0.54
1:B:143:MET:HA	1:B:143:MET:HE3	1.89	0.54
1:G:88:ARG:CA	1:G:89:THR:HB	2.17	0.54
1:G:187:THR:HG21	1:G:191:LYS:HB3	1.90	0.53
1:B:98:THR:HG22	1:B:133[A]:THR:HB	1.90	0.53
1:F:219:MET:HG2	1:F:237:ASP:OD1	2.10	0.52
1:H:198:VAL:O	1:H:202:GLU:HG2	2.10	0.52
1:E:128:THR:HB	1:E:129:PRO:HD2	1.90	0.52
1:G:87:PRO:O	1:G:88:ARG:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ILE:HG23	1:F:176:GLY:O	2.10	0.51
1:C:167:ALA:HA	1:C:177:ASP:O	2.10	0.51
1:H:109:THR:HG23	1:H:112:GLU:H	1.76	0.51
1:D:88:ARG:CZ	1:D:88:ARG:HB3	2.42	0.49
1:H:220:PHE:CD1	1:H:221:PRO:HD2	2.47	0.49
1:G:89:THR:O	1:G:89:THR:HG22	2.13	0.49
1:F:226:THR:CB	1:F:227:GLY:HA3	2.42	0.49
1:D:190:SER:HB3	1:D:225:TYR:CE2	2.48	0.49
1:E:211:HIS:CG	1:E:221:PRO:HG3	2.47	0.48
1:D:84:ASN:ND2	1:F:211:HIS:O	2.46	0.48
1:C:88:ARG:HB3	1:C:88:ARG:CZ	2.43	0.48
1:G:229:SER:O	1:G:230:HIS:HB3	2.14	0.47
1:E:135:LEU:HD12	1:E:140:ALA:HB2	1.96	0.47
1:G:229:SER:O	1:G:230:HIS:CB	2.62	0.47
1:A:96:ASN:ND2	1:B:213:LYS:O	2.47	0.47
5:C:3001:HAE:H13	6:C:4062:HOH:O	2.15	0.46
1:F:222:ILE:O	4:F:2006:GG1:H112	2.15	0.46
1:G:227:GLY:CA	1:G:228:LYS:HB3	2.23	0.46
1:E:238:VAL:O	1:E:242:GLN:HG3	2.15	0.46
1:C:89:THR:HA	1:E:88:ARG:HG3	1.97	0.46
1:D:228:LYS:HD3	6:D:4106:HOH:O	2.16	0.46
1:H:187:THR:HG21	1:H:191:LYS:HB3	1.97	0.46
1:C:135:LEU:HD21	1:D:222:ILE:HG12	1.98	0.46
1:H:220:PHE:O	4:H:2008:GG1:H16	2.16	0.45
1:F:125:SER:HB2	1:F:130:LEU:O	2.16	0.45
1:G:90:LEU:N	1:G:90:LEU:HD23	2.30	0.45
1:B:112:GLU:OE2	1:D:239:GLN:NE2	2.50	0.45
1:C:86:PHE:HE1	1:E:205:HIS:O	1.99	0.45
1:D:88:ARG:HA	1:F:90:LEU:HD21	1.99	0.44
1:F:242:GLN:HG2	1:F:247:PRO:HA	2.00	0.44
1:B:104:TYR:HB3	6:B:4049:HOH:O	2.17	0.44
1:D:87:PRO:O	1:F:90:LEU:HD22	2.18	0.44
1:C:88:ARG:C	1:E:88:ARG:HD3	2.37	0.44
1:H:242:GLN:HG2	1:H:247:PRO:HA	2.00	0.44
1:D:150:GLU:O	6:D:4129:HOH:O	2.21	0.44
1:C:191:LYS:O	1:C:192:GLY:C	2.56	0.44
1:H:142:ILE:HG23	1:H:176:GLY:O	2.18	0.43
1:C:191:LYS:HB3	1:C:191:LYS:HE2	1.77	0.43
1:H:128:THR:HB	1:H:129:PRO:CD	2.48	0.43
1:C:142:ILE:HG23	1:C:176:GLY:O	2.18	0.43
1:G:88:ARG:HG3	1:G:89:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:HIS:ND1	1:E:221:PRO:HG3	2.34	0.43
1:B:220:PHE:O	4:B:2002:GG1:H16	2.19	0.43
1:G:111[A]:SER:HB2	6:G:4097:HOH:O	2.18	0.43
1:E:237:ASP:O	1:E:241:ILE:HG22	2.19	0.43
1:E:239:GLN:CG	1:G:230:HIS:HB2	2.49	0.42
1:G:153:ASP:OD2	1:G:155:TYR:HB2	2.19	0.42
1:H:86:PHE:HB3	1:H:87:PRO:CD	2.50	0.42
1:H:88:ARG:CB	1:H:90:LEU:HG	2.46	0.42
1:C:86:PHE:CZ	1:E:169:PRO:HG3	2.54	0.42
1:G:233:LEU:HD12	1:G:234:PRO:HD2	2.01	0.42
1:B:135:LEU:HD12	1:B:140:ALA:HB2	2.02	0.42
1:E:214:ASP:HA	1:E:215:PRO:HD3	1.89	0.42
1:C:220:PHE:O	4:C:2003:GG1:H16	2.19	0.41
1:D:86:PHE:HE1	1:F:205:HIS:O	2.04	0.41
1:D:86:PHE:O	1:F:90:LEU:HD13	2.20	0.41
1:G:128:THR:HB	1:G:129:PRO:CD	2.51	0.41
1:F:88:ARG:HE	1:F:88:ARG:HB3	1.55	0.41
1:F:233:LEU:HA	1:F:234:PRO:HD3	1.94	0.41
1:F:212:SER:HB2	1:F:219:MET:O	2.21	0.40
1:D:99:TYR:HA	1:D:142:ILE:O	2.21	0.40
1:C:198:VAL:O	1:C:202:GLU:HG2	2.21	0.40
1:G:88:ARG:CG	1:G:89:THR:C	2.87	0.40
1:E:233:LEU:HD12	1:E:234:PRO:HD2	2.03	0.40
1:D:119:LYS:NZ	4:D:2004:GG1:O6	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:ND2	1:H:211:HIS:O[4_555]	1.92	0.28

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	165/170 (97%)	154 (93%)	10 (6%)	1 (1%)	30	36
1	B	165/170 (97%)	154 (93%)	10 (6%)	1 (1%)	30	36
1	C	165/170 (97%)	158 (96%)	6 (4%)	1 (1%)	30	36
1	D	164/170 (96%)	156 (95%)	8 (5%)	0	100	100
1	E	160/170 (94%)	150 (94%)	8 (5%)	2 (1%)	15	15
1	F	165/170 (97%)	150 (91%)	14 (8%)	1 (1%)	30	36
1	G	164/170 (96%)	154 (94%)	7 (4%)	3 (2%)	11	9
1	H	159/170 (94%)	146 (92%)	12 (8%)	1 (1%)	30	36
All	All	1307/1360 (96%)	1222 (94%)	75 (6%)	10 (1%)	24	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	240	GLY
1	E	248	GLY
1	F	248	GLY
1	G	90	LEU
1	G	230	HIS
1	A	228	LYS
1	B	161[A]	SER
1	C	90	LEU
1	G	88	ARG
1	H	85	VAL

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	142/144 (99%)	140 (99%)	2 (1%)	74	86
1	B	142/144 (99%)	135 (95%)	7 (5%)	31	41
1	C	142/144 (99%)	137 (96%)	5 (4%)	43	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	141/144 (98%)	137 (97%)	4 (3%)	51	68
1	E	139/144 (96%)	133 (96%)	6 (4%)	35	47
1	F	142/144 (99%)	135 (95%)	7 (5%)	31	41
1	G	141/144 (98%)	133 (94%)	8 (6%)	25	34
1	H	138/144 (96%)	132 (96%)	6 (4%)	35	47
All	All	1127/1152 (98%)	1082 (96%)	45 (4%)	38	52

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	182	ASP
1	B	88	ARG
1	B	90	LEU
1	B	115	LYS
1	B	143	MET
1	B	173	ASN
1	B	188	SER
1	B	232[A]	MET
1	C	88	ARG
1	C	91[A]	LYS
1	C	190	SER
1	C	224	THR
1	C	232[A]	MET
1	D	88	ARG
1	D	137	ASP
1	D	191	LYS
1	D	229	SER
1	E	91[A]	LYS
1	E	110	HIS
1	E	133[A]	THR
1	E	150	GLU
1	E	232[A]	MET
1	E	235[A]	ASP
1	F	89	THR
1	F	90	LEU
1	F	123	VAL
1	F	137	ASP
1	F	212	SER
1	F	229	SER

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Mol	Chain	Res	Type
1	F	232[A]	MET
1	G	90	LEU
1	G	118	LYS
1	G	131	ASN
1	G	133[A]	THR
1	G	150	GLU
1	G	188	SER
1	G	224	THR
1	G	229	SER
1	H	90	LEU
1	H	110	HIS
1	H	131	ASN
1	H	163	LEU
1	H	188	SER
1	H	213	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	B	131	ASN
1	B	173	ASN
1	C	110	HIS
1	G	84	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 52 ligands modelled in this entry, 40 are monoatomic - leaving 12 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
4	GG1	A	2001	-	28,35,35	1.57	3 (10%)	35,49,49	1.13	2 (5%)
4	GG1	B	2002	-	28,35,35	1.60	4 (14%)	35,49,49	1.17	2 (5%)
4	GG1	C	2003	-	28,35,35	1.62	3 (10%)	35,49,49	1.08	2 (5%)
5	HAE	C	3001	2	4,4,4	4.98	1 (25%)	4,4,4	0.84	0
4	GG1	D	2004	-	28,35,35	1.64	3 (10%)	35,49,49	0.93	1 (2%)
5	HAE	D	3002	2	4,4,4	4.63	1 (25%)	4,4,4	1.23	1 (25%)
4	GG1	E	2005	-	28,35,35	1.74	4 (14%)	35,49,49	1.04	2 (5%)
5	HAE	E	3003	2	4,4,4	4.74	1 (25%)	4,4,4	0.60	0
4	GG1	F	2006	-	28,35,35	1.61	3 (10%)	35,49,49	1.02	2 (5%)
5	HAE	F	3004	2	4,4,4	4.68	1 (25%)	4,4,4	1.57	1 (25%)
4	GG1	G	2007	-	28,35,35	1.76	5 (17%)	35,49,49	1.17	2 (5%)
4	GG1	H	2008	-	28,35,35	1.69	4 (14%)	35,49,49	0.99	1 (2%)

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
4	GG1	A	2001	-	-	0/10/14/14	0/4/4/4
4	GG1	B	2002	-	-	0/10/14/14	0/4/4/4
4	GG1	C	2003	-	-	0/10/14/14	0/4/4/4
5	HAE	C	3001	2	-	0/1/2/2	0/0/0/0
4	GG1	D	2004	-	-	0/10/14/14	0/4/4/4
5	HAE	D	3002	2	-	0/1/2/2	0/0/0/0
4	GG1	E	2005	-	-	1/10/14/14	0/4/4/4
5	HAE	E	3003	2	-	0/1/2/2	0/0/0/0
4	GG1	F	2006	-	-	1/10/14/14	0/4/4/4
5	HAE	F	3004	2	-	0/1/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GG1	G	2007	-	-	0/10/14/14	0/4/4/4
4	GG1	H	2008	-	-	0/10/14/14	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3001	HAE	O-N	-9.94	1.21	1.39
5	E	3003	HAE	O-N	-9.45	1.22	1.39
5	F	3004	HAE	O-N	-9.31	1.23	1.39
5	D	3002	HAE	O-N	-9.19	1.23	1.39
4	E	2005	GG1	C8-C7	-6.11	1.29	1.44
4	A	2001	GG1	C8-C7	-6.02	1.29	1.44
4	G	2007	GG1	C8-C7	-6.01	1.29	1.44
4	F	2006	GG1	C8-C7	-5.96	1.29	1.44
4	H	2008	GG1	C8-C7	-5.91	1.29	1.44
4	B	2002	GG1	C8-C7	-5.77	1.30	1.44
4	D	2004	GG1	C8-C7	-5.77	1.30	1.44
4	C	2003	GG1	C8-C7	-5.74	1.30	1.44
4	E	2005	GG1	C3-N1	-4.81	1.34	1.40
4	G	2007	GG1	C3-N1	-4.25	1.35	1.40
4	F	2006	GG1	C3-N1	-4.23	1.35	1.40
4	H	2008	GG1	C3-N1	-4.18	1.35	1.40
4	B	2002	GG1	C3-N1	-4.07	1.35	1.40
4	D	2004	GG1	C3-N1	-4.02	1.35	1.40
4	A	2001	GG1	C3-N1	-3.74	1.36	1.40
4	C	2003	GG1	C3-N1	-3.70	1.36	1.40
4	C	2003	GG1	C5-N6	-2.96	1.33	1.38
4	E	2005	GG1	C22-C3	-2.84	1.39	1.41
4	G	2007	GG1	C22-C3	-2.83	1.39	1.41
4	H	2008	GG1	C5-N6	-2.82	1.34	1.38
4	G	2007	GG1	C5-N6	-2.75	1.34	1.38
4	D	2004	GG1	C5-N6	-2.72	1.34	1.38
4	B	2002	GG1	C5-N6	-2.55	1.34	1.38
4	E	2005	GG1	C5-N6	-2.42	1.34	1.38
4	F	2006	GG1	C5-N6	-2.40	1.34	1.38
4	A	2001	GG1	C5-N6	-2.34	1.34	1.38
4	H	2008	GG1	C22-C3	-2.31	1.39	1.41
4	B	2002	GG1	C22-C3	-2.19	1.39	1.41
4	G	2007	GG1	C2-C6	2.04	1.40	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2005	GG1	C2-C3-N1	-2.27	120.03	121.78
4	F	2006	GG1	C25-N1-C3	2.27	121.20	118.11
4	G	2007	GG1	C4-N6-C1	2.35	120.84	118.05
5	D	3002	HAE	O-N-C2	2.36	123.20	119.86
5	F	3004	HAE	O-N-C2	3.01	124.12	119.86
4	C	2003	GG1	C25-N1-C3	3.06	122.29	118.11
4	F	2006	GG1	C22-C5-N6	3.48	118.97	116.09
4	A	2001	GG1	C25-N1-C3	3.49	122.88	118.11
4	A	2001	GG1	C22-C5-N6	3.62	119.08	116.09
4	C	2003	GG1	C22-C5-N6	3.80	119.23	116.09
4	B	2002	GG1	C25-N1-C3	3.84	123.35	118.11
4	B	2002	GG1	C22-C5-N6	4.00	119.39	116.09
4	D	2004	GG1	C22-C5-N6	4.12	119.49	116.09
4	E	2005	GG1	C22-C5-N6	4.46	119.77	116.09
4	H	2008	GG1	C22-C5-N6	4.47	119.78	116.09
4	G	2007	GG1	C22-C5-N6	5.11	120.31	116.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2005	GG1	C7-C26-C11-C20
4	F	2006	GG1	C7-C26-C11-C20

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	GG1	1	0
4	B	2002	GG1	1	0
4	C	2003	GG1	1	0
5	C	3001	HAE	1	0
4	D	2004	GG1	1	0
4	F	2006	GG1	1	0
4	H	2008	GG1	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	167/170 (98%)	-0.19	2 (1%) 81 85	12, 22, 37, 44	7 (4%)
1	B	167/170 (98%)	-0.15	2 (1%) 81 85	12, 22, 37, 44	7 (4%)
1	C	167/170 (98%)	-0.21	5 (2%) 54 63	12, 22, 37, 44	7 (4%)
1	D	166/170 (97%)	-0.21	2 (1%) 81 85	12, 22, 36, 44	7 (4%)
1	E	164/170 (96%)	0.14	6 (3%) 45 54	12, 23, 35, 44	7 (4%)
1	F	167/170 (98%)	0.21	6 (3%) 46 55	12, 23, 36, 44	6 (3%)
1	G	166/170 (97%)	0.12	7 (4%) 40 49	13, 23, 37, 44	7 (4%)
1	H	163/170 (95%)	0.01	5 (3%) 52 62	12, 23, 35, 44	6 (3%)
All	All	1327/1360 (97%)	-0.04	35 (2%) 59 68	12, 23, 37, 44	54 (4%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	89	THR	9.4
1	F	90	LEU	7.0
1	G	227	GLY	6.5
1	G	87	PRO	5.5
1	D	86	PHE	4.9
1	B	86	PHE	4.8
1	C	86	PHE	4.5
1	E	88	ARG	4.1
1	E	87	PRO	3.9
1	F	88	ARG	3.9
1	H	86	PHE	3.5
1	F	87	PRO	3.5
1	H	90	LEU	3.4
1	E	235[A]	ASP	3.2
1	A	86	PHE	3.0
1	G	90	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	230	HIS	2.9
1	E	247	PRO	2.8
1	H	87	PRO	2.8
1	C	85	VAL	2.7
1	F	240	GLY	2.7
1	G	88	ARG	2.7
1	B	249	ASP	2.6
1	C	87	PRO	2.6
1	H	88	ARG	2.5
1	F	96	ASN	2.4
1	H	85	VAL	2.4
1	E	249	ASP	2.3
1	C	84	ASN	2.3
1	E	96	ASN	2.3
1	C	83	TYR	2.1
1	D	88	ARG	2.1
1	G	92	TRP	2.1
1	F	230	HIS	2.0
1	A	249	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 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
5	HAE	D	3002	5/5	0.87	0.15	5.04	32,33,34,34	0
5	HAE	C	3001	5/5	0.89	0.14	2.18	28,30,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	HAE	F	3004	5/5	0.89	0.17	1.80	37,38,39,39	0
5	HAE	E	3003	5/5	0.89	0.15	0.55	39,41,41,41	0
4	GG1	E	2005	32/32	0.90	0.13	-0.04	32,33,34,34	0
4	GG1	A	2001	32/32	0.91	0.13	-0.19	19,21,22,23	0
4	GG1	B	2002	32/32	0.93	0.12	-0.42	17,20,21,22	0
4	GG1	H	2008	32/32	0.91	0.13	-0.45	20,23,26,28	0
4	GG1	G	2007	32/32	0.89	0.12	-0.46	21,22,25,26	0
4	GG1	F	2006	32/32	0.91	0.13	-0.49	26,27,30,31	0
2	ZN	B	4006	1/1	1.00	0.09	-0.57	19,19,19,19	0
3	CA	D	4020	1/1	0.97	0.09	-0.71	40,40,40,40	0
4	GG1	C	2003	32/32	0.94	0.11	-0.73	9,14,14,15	0
4	GG1	D	2004	32/32	0.95	0.10	-0.83	15,17,18,18	0
3	CA	H	4039	1/1	0.95	0.08	-1.20	33,33,33,33	0
3	CA	E	4025	1/1	0.97	0.07	-1.21	39,39,39,39	0
3	CA	F	4028	1/1	0.95	0.07	-1.80	30,30,30,30	0
3	CA	G	4035	1/1	0.92	0.07	-1.86	51,51,51,51	0
2	ZN	A	4001	1/1	1.00	0.10	-2.00	18,18,18,18	0
3	CA	C	4013	1/1	0.98	0.08	-2.06	17,17,17,17	0
3	CA	D	4018	1/1	0.99	0.05	-2.10	20,20,20,20	0
3	CA	G	4034	1/1	0.94	0.06	-2.16	43,43,43,43	0
2	ZN	F	4027	1/1	0.99	0.09	-2.25	23,23,23,23	0
2	ZN	A	4002	1/1	1.00	0.09	-2.30	19,19,19,19	0
3	CA	A	4005	1/1	0.98	0.05	-2.31	41,41,41,41	0
2	ZN	E	4022	1/1	0.99	0.07	-2.31	23,23,23,23	0
2	ZN	D	4017	1/1	0.99	0.07	-2.41	18,18,18,18	0
3	CA	F	4029	1/1	0.91	0.06	-2.42	36,36,36,36	0
3	CA	E	4024	1/1	0.96	0.05	-2.53	36,36,36,36	0
3	CA	F	4030	1/1	0.96	0.06	-2.63	37,37,37,37	0
2	ZN	D	4016	1/1	1.00	0.08	-2.71	16,16,16,16	0
3	CA	A	4004	1/1	0.97	0.04	-2.79	28,28,28,28	0
3	CA	B	4010	1/1	0.98	0.05	-2.90	44,44,44,44	0
2	ZN	G	4032	1/1	0.98	0.07	-2.96	24,24,24,24	0
3	CA	E	4023	1/1	0.99	0.04	-2.98	23,23,23,23	0
3	CA	B	4009	1/1	0.99	0.04	-3.02	28,28,28,28	0
3	CA	B	4008	1/1	1.00	0.05	-3.08	19,19,19,19	0
2	ZN	C	4011	1/1	1.00	0.07	-3.45	17,17,17,17	0
3	CA	C	4014	1/1	0.98	0.03	-3.53	26,26,26,26	0
3	CA	D	4019	1/1	0.99	0.02	-3.85	26,26,26,26	0
2	ZN	B	4007	1/1	0.99	0.08	-3.92	20,20,20,20	0
2	ZN	H	4037	1/1	0.98	0.07	-4.01	26,26,26,26	0
3	CA	H	4040	1/1	0.95	0.04	-4.42	46,46,46,46	0
2	ZN	C	4012	1/1	1.00	0.06	-4.78	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	A	4003	1/1	0.99	0.04	-5.05	18,18,18,18	0
3	CA	H	4038	1/1	0.98	0.05	-5.14	30,30,30,30	0
3	CA	C	4015	1/1	0.98	0.05	-5.92	36,36,36,36	0
3	CA	G	4033	1/1	0.98	0.04	-7.85	26,26,26,26	0
2	ZN	F	4026	1/1	0.97	0.06	-	44,44,44,44	0
2	ZN	E	4021	1/1	0.98	0.06	-	34,34,34,34	0
2	ZN	H	4036	1/1	0.96	0.12	-	31,31,31,31	0
2	ZN	G	4031	1/1	0.96	0.11	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.