Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:10 PM GMT

PDB ID	:	4BOF
Title	:	Crystal structure of arginine deiminase from group A streptococcus
Authors	:	Henningham, A.; Ericsson, D.J.; Langer, K.; Casey, L.; Jovcevski, B.; Chhatwal, G.S.; Aquilina, J.A.; Batzloff, M.R.; Kobe, B.; Walker, M.J.
Deposited on	:	2013-05-20
Resolution	:	2.48 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 ①) were used in the production of this report:

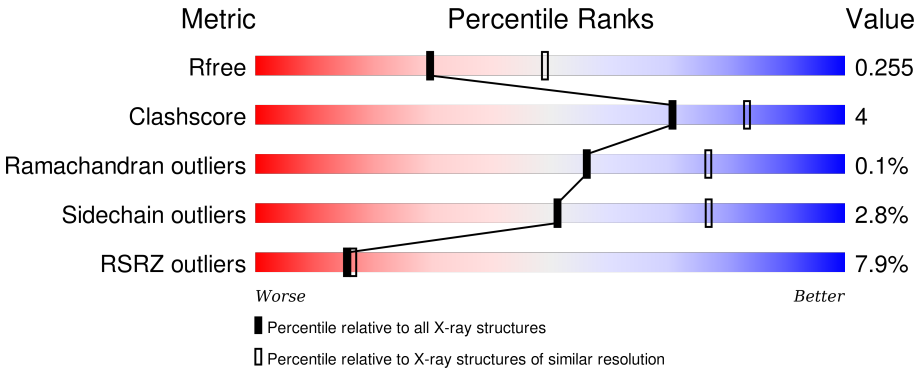
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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 <=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	411	3% 87% 11%
1	B	411	5% 91% 9%
1	C	411	3% 89% 9%
1	D	411	3% 89% 10%
1	E	411	19% 88% 11%

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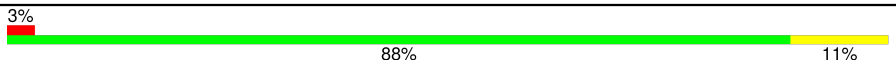
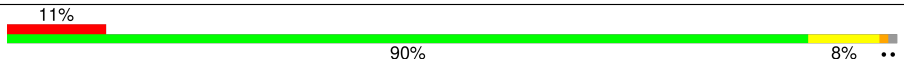
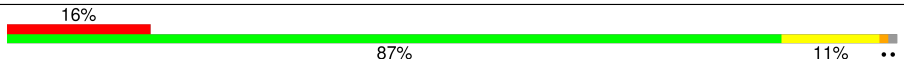
Mol	Chain	Length	Quality of chain
1	F	411	
1	G	411	
1	H	411	

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	SO4	A	420	-	-	X	X
2	SO4	B	420	-	-	X	X
2	SO4	C	420	-	-	X	X
2	SO4	D	420	-	-	X	X
2	SO4	E	420	-	-	X	X
2	SO4	F	420	-	-	X	-
2	SO4	G	420	-	-	X	X
2	SO4	H	420	-	-	-	X
2	SO4	H	421	-	-	-	X
3	PGE	A	422	-	-	X	X
3	PGE	F	423	-	-	-	X
4	PG4	F	422	-	-	X	-

2 Entry composition (i)

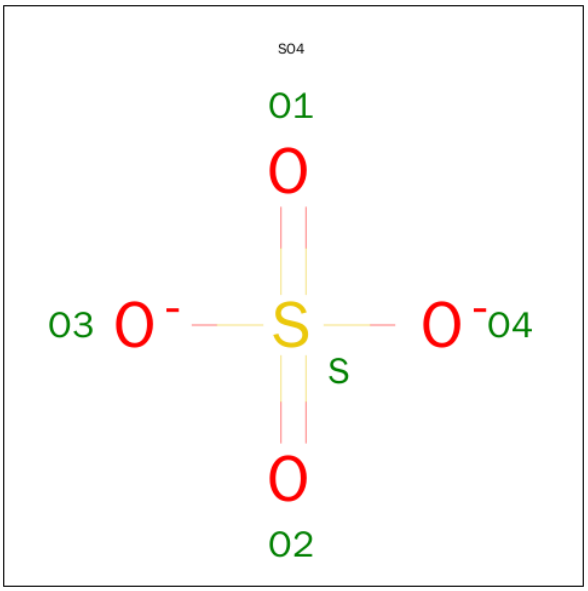
There are 5 unique types of molecules in this entry. The entry contains 26319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ARGININE DEIMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3237	2055	547	623	12			
1	B	411	Total	C	N	O	S	0	0	0
			3257	2067	550	627	13			
1	C	409	Total	C	N	O	S	0	0	0
			3242	2058	548	624	12			
1	D	409	Total	C	N	O	S	0	0	0
			3242	2058	548	624	12			
1	E	406	Total	C	N	O	S	0	0	0
			3221	2046	544	619	12			
1	F	409	Total	C	N	O	S	0	0	0
			3242	2058	548	624	12			
1	G	408	Total	C	N	O	S	0	0	0
			3237	2055	547	623	12			
1	H	408	Total	C	N	O	S	0	0	0
			3237	2055	547	623	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

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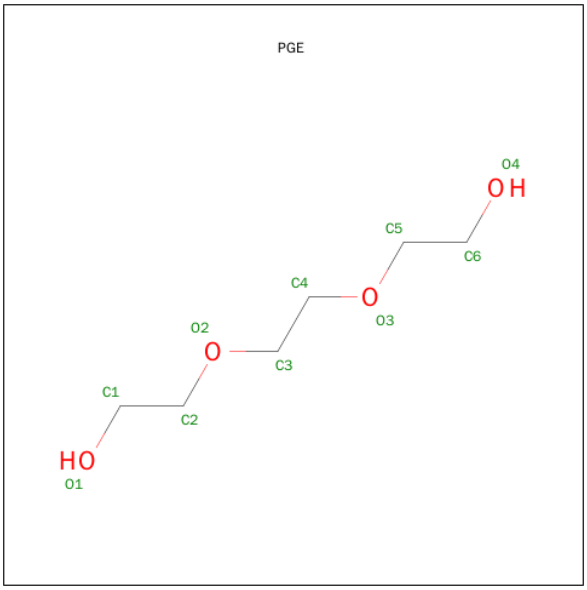
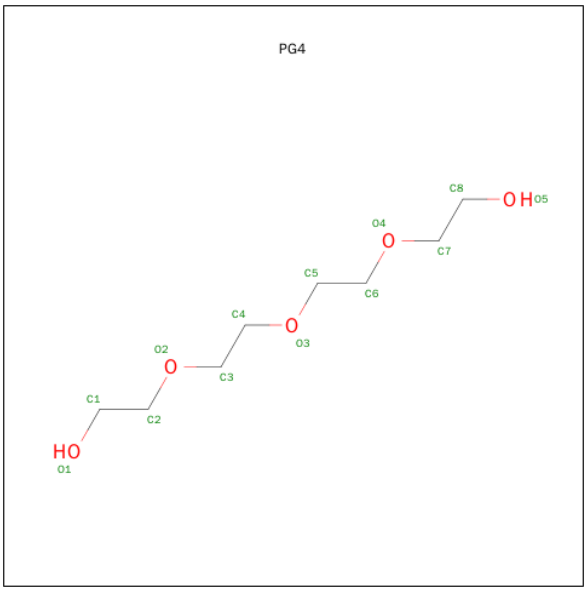
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	F	1	Total C O 10 6 4	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 13 8 5	0	0

- Molecule 5 is water.

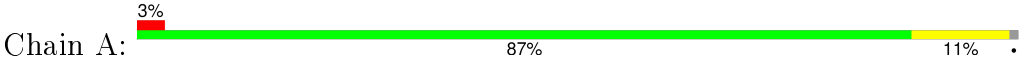
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0
5	B	20	Total O 20 20	0	0
5	C	49	Total O 49 49	0	0
5	D	41	Total O 41 41	0	0
5	E	7	Total O 7 7	0	0
5	F	62	Total O 62 62	0	0
5	G	20	Total O 20 20	0	0
5	H	25	Total O 25 25	0	0

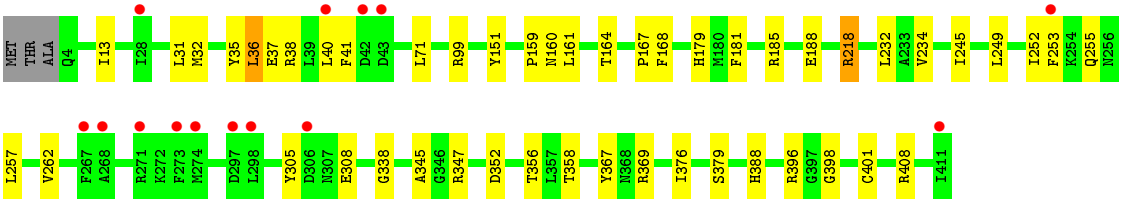
3 Residue-property plots (i)

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: ARGININE DEIMINASE

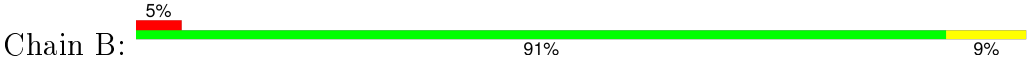
Chain A:

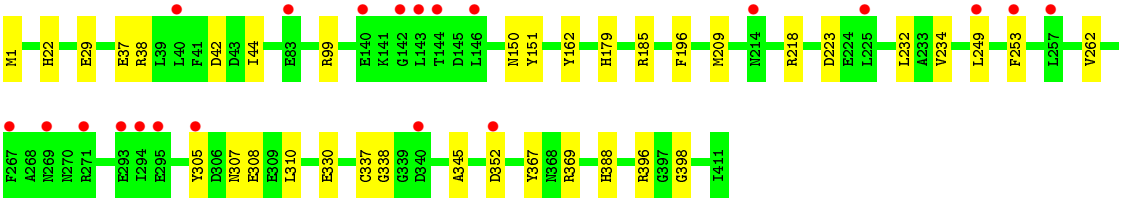




- Molecule 1: ARGININE DEIMINASE

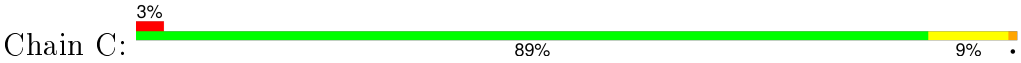
Chain B:

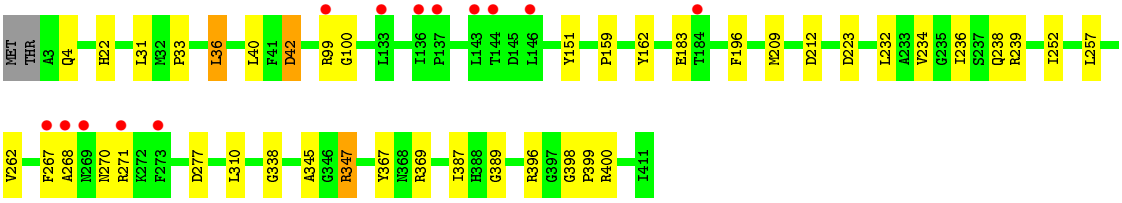




- Molecule 1: ARGININE DEIMINASE

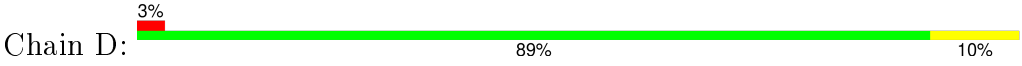
Chain C:

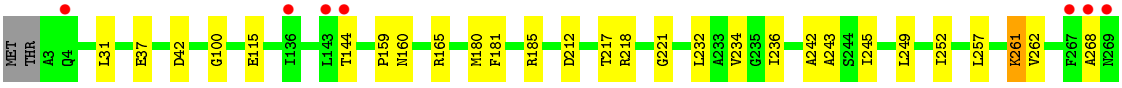




- Molecule 1: ARGININE DEIMINASE

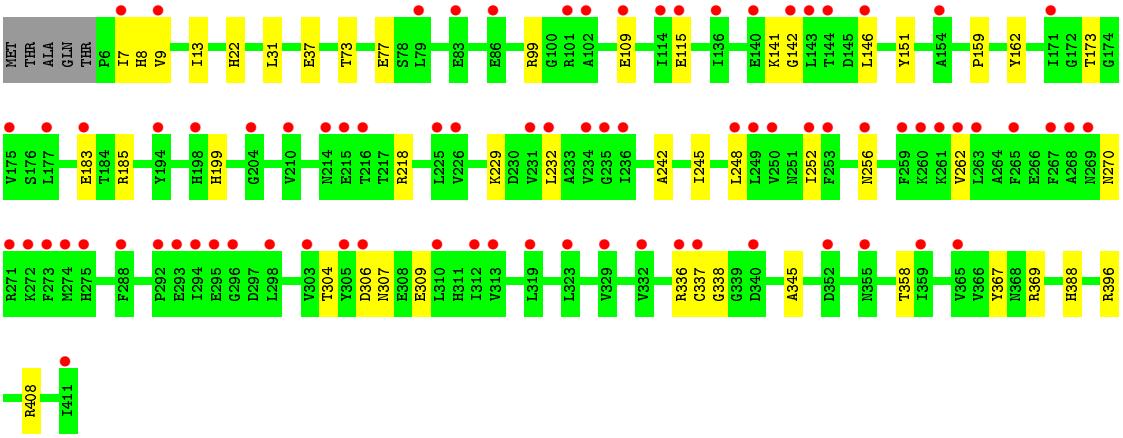
Chain D:





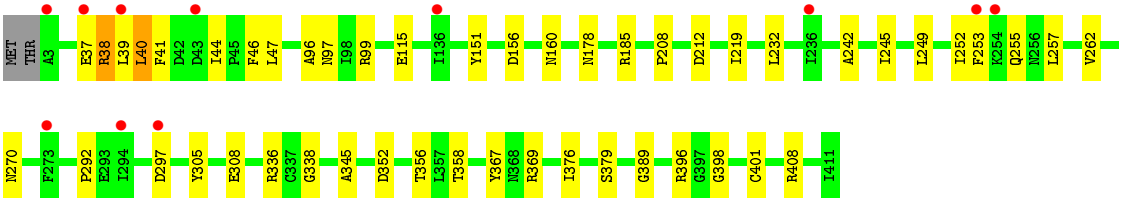
• Molecule 1: ARGININE DEIMINASE

Chain E:



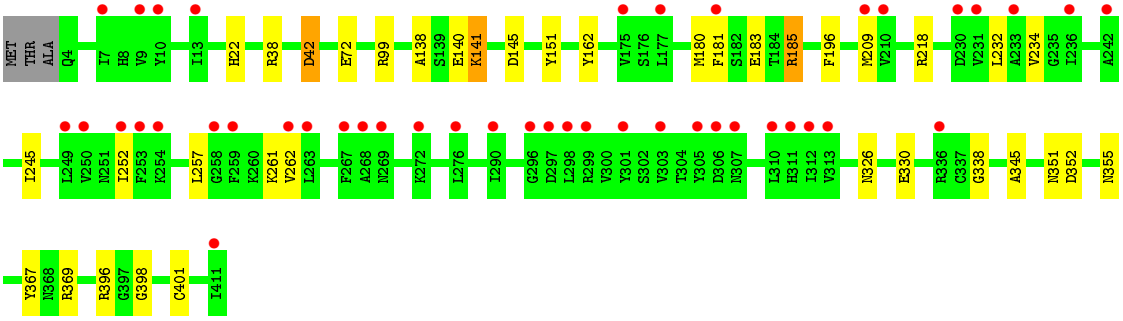
• Molecule 1: ARGININE DEIMINASE

Chain F:



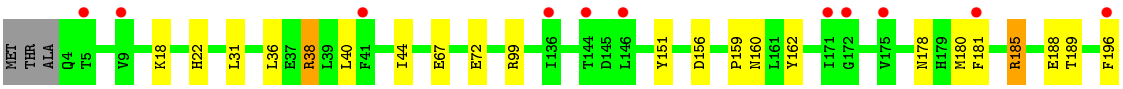
• Molecule 1: ARGININE DEIMINASE

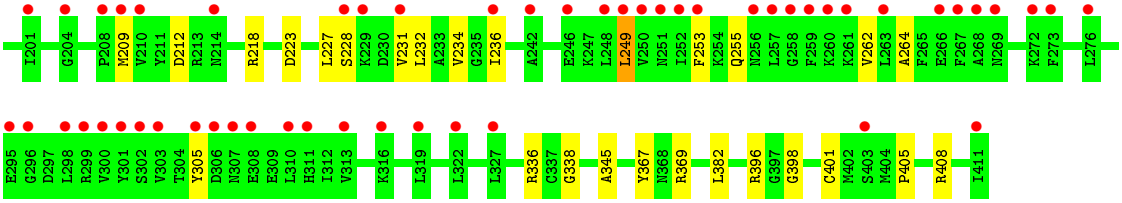
Chain G:



• Molecule 1: ARGININE DEIMINASE

Chain H:




I201
G204
P208
M209
V210
Y211
D212
R213
N214
R218
D223
L227
S228
K229
D230
V231
L232
A233
V234
G235
I236
A242
E246
K247
L248
L249
V250
N251
I252
F253
K254
Q255
N256
L257
G258
F259
K260
K261
V262
L263
A264
F265
E266
F267
A268
N269
K272
F273
L276
E295
G296
D297
L298
R299
V300
Y301
S302
V303
T304
Y305
D306
N307
E308
E309
L310
H311
I312
V313
K316
L319
L322
L327
R336
G337
G338
A345
Y367
N368
R369
L382
R396
G397
G398
C401
M402
S403
M404
P405
R408
I411

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	87.91Å 92.74Å 120.97Å 96.15° 90.27° 100.13°	Depositor
Resolution (Å)	36.31 – 2.48 61.60 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.31-2.48) 96.3 (61.60-2.48)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.211 , 0.244 0.222 , 0.255	Depositor DCC
R_{free} test set	6579 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 131658 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26319	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, PGE, SO4

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	0.54	0/3296	0.70	0/4457
1	B	0.47	0/3316	0.65	0/4484
1	C	0.52	0/3301	0.69	1/4464 (0.0%)
1	D	0.52	0/3301	0.68	0/4464
1	E	0.47	0/3280	0.66	0/4434
1	F	0.54	0/3301	0.70	0/4464
1	G	0.48	0/3296	0.65	0/4457
1	H	0.47	0/3296	0.65	0/4457
All	All	0.50	0/26387	0.67	1/35681 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	GLN	C-N-CA	5.53	135.52	121.70

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	3237	0	3231	48	0
1	B	3257	0	3255	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3242	0	3236	25	0
1	D	3242	0	3236	23	0
1	E	3221	0	3217	22	0
1	F	3242	0	3236	41	0
1	G	3237	0	3231	25	0
1	H	3237	0	3231	29	0
2	A	10	0	0	2	0
2	B	10	0	0	3	0
2	C	10	0	0	4	0
2	D	10	0	0	2	0
2	E	10	0	0	3	0
2	F	10	0	0	4	0
2	G	10	0	0	3	0
2	H	10	0	0	1	0
3	A	10	0	14	20	0
3	F	10	0	14	4	0
4	F	13	0	18	14	0
5	A	67	0	0	3	0
5	B	20	0	0	0	0
5	C	49	0	0	1	0
5	D	41	0	0	1	0
5	E	7	0	0	0	0
5	F	62	0	0	2	0
5	G	20	0	0	0	0
5	H	25	0	0	2	0
All	All	26319	0	25919	226	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 (226) 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:H:369:ARG:HD2	2:H:420:SO4:O3	1.56	1.03
1:A:167:PRO:HG2	3:A:422:PGE:H52	1.47	0.97
1:A:249:LEU:HD22	1:A:262:VAL:HG21	1.46	0.95
1:G:369:ARG:HD2	2:G:420:SO4:O3	1.67	0.95
1:F:249:LEU:HD22	1:F:262:VAL:HG21	1.48	0.93
4:F:422:PG4:H21	1:G:369:ARG:HH21	1.32	0.93
1:A:167:PRO:HB2	3:A:422:PGE:H22	1.50	0.91
1:A:245:ILE:O	1:A:249:LEU:HG	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:GLY:O	1:E:146:LEU:HD13	1.76	0.85
1:A:188:GLU:OE1	3:A:422:PGE:H62	1.75	0.85
1:B:179:HIS:HD2	1:B:218:ARG:HD3	1.40	0.83
1:F:358:THR:O	1:F:408:ARG:NH2	2.11	0.83
1:C:389:GLY:N	2:C:420:SO4:O3	2.09	0.83
1:F:44:ILE:O	4:F:422:PG4:H12	1.80	0.81
1:C:267:PHE:HB2	1:C:270:ASN:HD22	1.46	0.80
1:A:164:THR:HA	3:A:422:PGE:H3	1.66	0.78
1:B:179:HIS:CD2	1:B:218:ARG:HD3	2.21	0.76
1:F:369:ARG:NH1	2:F:420:SO4:O4	2.18	0.75
1:A:168:PHE:CE2	3:A:422:PGE:H2	2.22	0.75
1:F:46:PHE:HD1	4:F:422:PG4:H51	1.51	0.74
1:A:167:PRO:CG	3:A:422:PGE:H52	2.16	0.74
1:D:369:ARG:HB3	2:D:420:SO4:O2	1.88	0.74
4:F:422:PG4:H31	1:G:351:ASN:ND2	2.04	0.72
1:A:388:HIS:HA	2:A:420:SO4:O1	1.90	0.72
1:B:369:ARG:HB3	2:B:420:SO4:O3	1.90	0.72
1:E:141:LYS:HB3	1:E:146:LEU:HD12	1.73	0.71
1:F:245:ILE:O	1:F:249:LEU:HG	1.91	0.69
1:C:369:ARG:NH1	2:C:420:SO4:O2	2.25	0.69
1:H:180:MET:HE3	1:H:185:ARG:HG2	1.75	0.67
1:F:47:LEU:H	4:F:422:PG4:H62	1.58	0.67
1:A:356:THR:HA	5:A:2060:HOH:O	1.96	0.66
1:F:46:PHE:CD1	4:F:422:PG4:H51	2.31	0.65
1:H:181:PHE:HA	1:H:218:ARG:HD2	1.79	0.65
1:D:252:ILE:HG23	1:D:257:LEU:HB2	1.79	0.65
1:F:356:THR:HA	5:F:2051:HOH:O	1.96	0.64
1:D:236:ILE:HG22	1:D:268:ALA:HB2	1.80	0.64
1:C:196:PHE:HB3	1:C:209:MET:HE3	1.80	0.63
1:A:358:THR:O	1:A:408:ARG:NH2	2.26	0.63
1:C:196:PHE:HB3	1:C:209:MET:CE	2.29	0.63
1:F:369:ARG:N	2:F:420:SO4:O2	2.27	0.62
1:C:252:ILE:HG23	1:C:257:LEU:HB2	1.81	0.62
1:E:141:LYS:HB3	1:E:146:LEU:CD1	2.29	0.62
1:E:369:ARG:HB3	2:E:420:SO4:O1	1.99	0.62
1:A:167:PRO:HG2	3:A:422:PGE:C5	2.28	0.62
1:G:181:PHE:HA	1:G:218:ARG:HD2	1.82	0.62
1:A:167:PRO:HG2	3:A:422:PGE:H32	1.82	0.61
1:E:388:HIS:HA	2:E:420:SO4:O2	2.01	0.61
1:H:196:PHE:HB3	1:H:209:MET:CE	2.30	0.61
1:F:44:ILE:O	4:F:422:PG4:C1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:422:PG4:H22	1:G:369:ARG:HE	1.66	0.61
1:D:291:HIS:CE1	1:D:293:GLU:HB2	2.37	0.60
1:G:196:PHE:HB3	1:G:209:MET:HE3	1.84	0.60
1:H:227:LEU:HB2	1:H:231:VAL:HG13	1.83	0.59
1:D:181:PHE:HA	1:D:218:ARG:HD2	1.82	0.59
1:G:138:ALA:HA	1:G:141:LYS:HD3	1.84	0.59
1:F:292:PRO:HB3	1:F:336:ARG:HE	1.68	0.59
1:B:196:PHE:HB3	1:B:209:MET:CE	2.32	0.59
1:A:168:PHE:CD2	3:A:422:PGE:H2	2.38	0.59
1:D:348:GLU:HG2	1:D:370:ASN:HD22	1.68	0.58
1:D:261:LYS:HG3	1:D:304:THR:HG22	1.83	0.58
1:G:22:HIS:HB3	1:G:162:TYR:HA	1.85	0.58
1:B:196:PHE:HB3	1:B:209:MET:HE3	1.83	0.58
1:A:181:PHE:HA	1:A:218:ARG:HG2	1.84	0.58
1:A:179:HIS:HD2	1:A:218:ARG:HG3	1.68	0.58
1:D:234:VAL:HG21	1:D:245:ILE:HG12	1.85	0.58
1:A:347:ARG:HG2	1:H:44:ILE:HG21	1.84	0.57
1:E:183:GLU:HG2	1:E:218:ARG:HH12	1.69	0.57
1:H:236:ILE:HD11	1:H:264:ALA:HB1	1.86	0.57
1:G:196:PHE:HB3	1:G:209:MET:CE	2.35	0.57
1:H:180:MET:CE	1:H:185:ARG:HG2	2.34	0.56
1:G:141:LYS:HG2	1:G:145:ASP:HB3	1.87	0.56
1:A:160:ASN:O	3:A:422:PGE:H6	2.06	0.56
1:C:369:ARG:HB3	2:C:420:SO4:O2	2.04	0.56
1:G:232:LEU:HB2	1:G:262:VAL:HG22	1.87	0.56
1:E:77:GLU:HB2	1:E:199:HIS:HE1	1.70	0.56
1:A:232:LEU:HB2	1:A:262:VAL:HG22	1.88	0.55
1:E:22:HIS:HB3	1:E:162:TYR:HA	1.88	0.55
1:G:180:MET:HE3	1:G:185:ARG:HG2	1.88	0.55
1:F:369:ARG:HD2	2:F:420:SO4:O4	2.06	0.54
1:H:40:LEU:O	5:H:2006:HOH:O	2.18	0.54
1:C:238:GLN:HG3	1:C:239:ARG:HG2	1.89	0.54
1:A:167:PRO:CB	3:A:422:PGE:H22	2.32	0.54
1:C:40:LEU:O	5:C:2010:HOH:O	2.18	0.54
1:B:249:LEU:HD11	1:B:253:PHE:HE1	1.73	0.54
1:A:188:GLU:OE1	3:A:422:PGE:C6	2.54	0.54
1:E:77:GLU:HB2	1:E:199:HIS:CE1	2.43	0.54
1:F:232:LEU:HB2	1:F:262:VAL:HG22	1.90	0.53
1:H:232:LEU:HB2	1:H:262:VAL:HG22	1.89	0.53
1:A:249:LEU:O	1:A:253:PHE:HD2	1.92	0.53
1:E:367:TYR:HB3	2:E:420:SO4:O3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ILE:O	4:F:422:PG4:C2	2.57	0.53
1:A:185:ARG:HH21	3:A:422:PGE:H62	1.73	0.53
1:B:232:LEU:HB2	1:B:262:VAL:HG22	1.89	0.53
1:C:277:ASP:OD2	1:C:400:ARG:NH1	2.42	0.53
1:B:44:ILE:HG21	1:C:347:ARG:HG2	1.91	0.52
1:A:161:LEU:HA	3:A:422:PGE:H5	1.92	0.52
1:D:232:LEU:HB2	1:D:262:VAL:HG22	1.90	0.52
1:C:236:ILE:HG22	1:C:268:ALA:HB2	1.91	0.52
1:H:22:HIS:HB3	1:H:162:TYR:HA	1.91	0.52
1:A:160:ASN:ND2	5:A:2011:HOH:O	2.36	0.51
1:H:249:LEU:O	1:H:253:PHE:HD1	1.91	0.51
1:F:389:GLY:N	2:F:420:SO4:O1	2.43	0.51
1:A:249:LEU:CD2	1:A:262:VAL:HG21	2.32	0.51
1:F:156:ASP:CB	3:F:423:PGE:H6	2.41	0.51
1:F:249:LEU:O	1:F:253:PHE:HD2	1.94	0.51
1:C:232:LEU:HB2	1:C:262:VAL:HG22	1.93	0.51
1:H:196:PHE:HB3	1:H:209:MET:HE3	1.92	0.50
1:D:242:ALA:HA	1:D:245:ILE:HD12	1.93	0.50
1:A:185:ARG:HH21	3:A:422:PGE:C6	2.25	0.50
1:F:252:ILE:HG23	1:F:257:LEU:HB2	1.94	0.50
1:G:234:VAL:HG21	1:G:245:ILE:HG23	1.94	0.50
1:G:369:ARG:NH1	2:G:420:SO4:O3	2.32	0.50
1:B:99:ARG:HH22	1:B:151:TYR:HB3	1.77	0.50
1:E:232:LEU:HB2	1:E:262:VAL:HG22	1.93	0.50
1:A:167:PRO:CG	3:A:422:PGE:H32	2.41	0.49
1:D:368:ASN:N	2:D:420:SO4:O1	2.45	0.49
1:F:249:LEU:CD2	1:F:262:VAL:HG21	2.33	0.49
4:F:422:PG4:H21	1:G:369:ARG:NH2	2.15	0.49
1:A:252:ILE:HG23	1:A:257:LEU:HB2	1.94	0.49
1:H:228:SER:OG	1:H:231:VAL:HG12	2.13	0.48
1:A:99:ARG:HH22	1:A:151:TYR:HB3	1.77	0.48
1:G:99:ARG:HH22	1:G:151:TYR:HB3	1.78	0.48
1:F:156:ASP:HB3	3:F:423:PGE:H6	1.94	0.48
1:G:38:ARG:NH2	1:G:151:TYR:OH	2.46	0.48
1:F:305:TYR:CE2	1:F:308:GLU:HA	2.48	0.48
1:F:99:ARG:HH22	1:F:151:TYR:HB3	1.77	0.48
1:H:99:ARG:HH22	1:H:151:TYR:HB3	1.79	0.48
1:B:249:LEU:CD1	1:B:253:PHE:HE1	2.26	0.48
1:H:196:PHE:HB3	1:H:209:MET:HE1	1.96	0.48
1:D:351:ASN:HB2	1:D:370:ASN:HD21	1.78	0.47
1:D:261:LYS:HG3	1:D:304:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ARG:HH22	1:E:151:TYR:HB3	1.79	0.47
1:C:99:ARG:HH22	1:C:151:TYR:HB3	1.78	0.47
1:A:379:SER:HB2	1:F:376:ILE:HG13	1.95	0.47
1:G:42:ASP:OD1	1:G:396:ARG:HG2	2.14	0.47
1:A:367:TYR:CE2	1:A:398:GLY:HA2	2.50	0.47
1:F:338:GLY:HA3	1:F:345:ALA:HA	1.96	0.47
1:A:71:LEU:HD11	3:A:422:PGE:H12	1.96	0.47
1:E:13:ILE:HG22	1:E:358:THR:HG21	1.97	0.47
1:B:305:TYR:HD1	1:B:310:LEU:HG	1.80	0.47
1:F:242:ALA:HA	1:F:245:ILE:HD12	1.96	0.47
1:A:379:SER:HB2	1:F:376:ILE:CG1	2.45	0.47
1:E:338:GLY:HA3	1:E:345:ALA:HA	1.97	0.47
1:A:31:LEU:HD21	1:A:159:PRO:HG3	1.98	0.46
1:H:38:ARG:NH2	1:H:156:ASP:OD2	2.49	0.46
1:C:100:GLY:HA2	2:C:421:SO4:O1	2.16	0.46
1:C:223:ASP:O	1:C:234:VAL:HA	2.16	0.46
1:F:249:LEU:O	1:F:253:PHE:CD2	2.68	0.46
1:E:248:LEU:HG	1:E:252:ILE:HD12	1.98	0.46
1:E:77:GLU:CB	1:E:199:HIS:CE1	2.99	0.45
1:F:37:GLU:HG3	1:F:38:ARG:N	2.31	0.45
1:F:160:ASN:ND2	5:F:2013:HOH:O	2.42	0.45
1:H:338:GLY:HA3	1:H:345:ALA:HA	1.98	0.45
1:F:367:TYR:CE2	1:F:398:GLY:HA2	2.52	0.45
1:F:46:PHE:HA	4:F:422:PG4:H41	1.97	0.45
1:D:367:TYR:CE2	1:D:398:GLY:HA2	2.51	0.45
1:A:161:LEU:HA	3:A:422:PGE:C5	2.46	0.45
1:F:208:PRO:HB3	1:F:255:GLN:HG2	1.98	0.45
1:C:42:ASP:OD1	1:C:396:ARG:HG2	2.17	0.45
1:H:38:ARG:C	1:H:40:LEU:H	2.20	0.45
1:E:77:GLU:CB	1:E:199:HIS:HE1	2.30	0.45
1:G:261:LYS:NZ	1:G:326:ASN:HD21	2.15	0.45
1:G:369:ARG:N	2:G:420:SO4:O4	2.50	0.45
1:H:367:TYR:CE2	1:H:398:GLY:HA2	2.52	0.45
1:B:367:TYR:CE2	1:B:398:GLY:HA2	2.53	0.44
1:E:9:VAL:HG22	1:E:408:ARG:HG3	1.98	0.44
1:A:32:MET:O	1:A:36:LEU:HD13	2.16	0.44
1:F:96:ALA:O	3:F:423:PGE:H32	2.17	0.44
1:F:97:ASN:HD22	3:F:423:PGE:H4	1.82	0.44
1:A:249:LEU:O	1:A:253:PHE:CD2	2.69	0.44
1:H:223:ASP:O	1:H:234:VAL:HA	2.18	0.44
1:B:223:ASP:O	1:B:234:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:HIS:HB3	1:B:162:TYR:HA	1.99	0.44
1:A:305:TYR:CE2	1:A:308:GLU:HA	2.53	0.44
1:D:180:MET:HE3	1:D:185:ARG:HB3	2.00	0.44
1:B:338:GLY:HA3	1:B:345:ALA:HA	1.99	0.44
1:F:178:ASN:HB3	1:F:219:ILE:O	2.18	0.43
1:D:100:GLY:HA2	1:D:144:THR:HG23	2.00	0.43
1:C:367:TYR:CE2	1:C:398:GLY:HA2	2.53	0.43
1:G:338:GLY:HA3	1:G:345:ALA:HA	2.00	0.43
1:D:234:VAL:CG2	1:D:245:ILE:HG12	2.46	0.43
1:C:33:PRO:HA	1:C:36:LEU:HD22	2.00	0.43
1:G:352:ASP:HB3	1:G:355:ASN:HB3	2.00	0.43
1:C:387:ILE:HD11	1:C:399:PRO:HG3	2.00	0.43
1:H:253:PHE:CD2	1:H:305:TYR:HB3	2.54	0.43
1:H:178:ASN:O	1:H:189:THR:HG21	2.19	0.43
1:A:161:LEU:HD23	3:A:422:PGE:H4	2.00	0.43
1:F:37:GLU:HG3	1:F:38:ARG:H	1.84	0.43
1:G:367:TYR:CE2	1:G:398:GLY:HA2	2.53	0.42
1:D:285:TYR:CE1	1:D:411:ILE:HD12	2.54	0.42
1:D:165:ARG:O	1:D:221:GLY:HA3	2.19	0.42
1:C:22:HIS:HB3	1:C:162:TYR:HA	2.00	0.42
1:B:367:TYR:HB3	2:B:420:SO4:O1	2.18	0.42
1:E:306:ASP:O	1:E:309:GLU:HG2	2.19	0.42
1:A:234:VAL:HG21	1:A:245:ILE:HG23	2.00	0.42
1:H:185:ARG:NH1	1:H:188:GLU:OE1	2.52	0.42
1:A:13:ILE:HG22	1:A:358:THR:HG21	2.00	0.42
1:B:29:GLU:O	1:C:347:ARG:HD3	2.19	0.42
1:A:160:ASN:C	3:A:422:PGE:H6	2.40	0.42
1:B:388:HIS:HA	2:B:420:SO4:O4	2.20	0.42
1:A:356:THR:HG22	5:A:2058:HOH:O	2.20	0.42
1:F:44:ILE:O	4:F:422:PG4:O2	2.38	0.42
1:H:249:LEU:HD11	1:H:262:VAL:HG11	2.01	0.42
1:F:38:ARG:C	1:F:40:LEU:H	2.23	0.42
1:D:160:ASN:ND2	5:D:2011:HOH:O	2.53	0.41
1:H:31:LEU:HD21	1:H:159:PRO:HG3	2.01	0.41
1:C:367:TYR:CE1	1:C:389:GLY:HA3	2.55	0.41
1:E:7:ILE:O	1:E:173:THR:HA	2.20	0.41
1:E:242:ALA:HA	1:E:245:ILE:HD12	2.02	0.41
1:C:31:LEU:HD21	1:C:159:PRO:HG3	2.02	0.41
1:F:47:LEU:HB3	4:F:422:PG4:H71	2.02	0.41
1:A:369:ARG:HD2	2:A:420:SO4:O3	2.21	0.41
1:H:18:LYS:HG2	1:H:67:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ILE:HG13	1:F:379:SER:HB2	2.01	0.41
4:F:422:PG4:H11	1:G:351:ASN:OD1	2.21	0.41
1:D:31:LEU:HD21	1:D:159:PRO:HG3	2.02	0.41
1:H:160:ASN:ND2	5:H:2006:HOH:O	2.50	0.40
1:D:217:THR:HG21	1:D:243:ALA:HB3	2.03	0.40
1:A:35:TYR:HB3	1:A:38:ARG:HG2	2.03	0.40
1:A:338:GLY:HA3	1:A:345:ALA:HA	2.03	0.40
1:B:305:TYR:CE2	1:B:308:GLU:HA	2.56	0.40
1:D:285:TYR:HE1	1:D:411:ILE:HD12	1.85	0.40
1:H:405:PRO:HG2	1:H:408:ARG:NH1	2.36	0.40
1:G:252:ILE:HG23	1:G:257:LEU:HB2	2.04	0.40
1:E:31:LEU:HD21	1:E:159:PRO:HG3	2.04	0.40
1:C:338:GLY:HA3	1:C:345:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/411 (99%)	389 (96%)	17 (4%)	0	100	100
1	B	409/411 (100%)	396 (97%)	12 (3%)	1 (0%)	52	73
1	C	407/411 (99%)	395 (97%)	12 (3%)	0	100	100
1	D	407/411 (99%)	396 (97%)	11 (3%)	0	100	100
1	E	404/411 (98%)	387 (96%)	17 (4%)	0	100	100
1	F	407/411 (99%)	386 (95%)	20 (5%)	1 (0%)	52	73
1	G	406/411 (99%)	394 (97%)	12 (3%)	0	100	100
1	H	406/411 (99%)	395 (97%)	11 (3%)	0	100	100
All	All	3252/3288 (99%)	3138 (96%)	112 (3%)	2 (0%)	56	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	307	ASN
1	F	39	LEU

5.3.2 Protein sidechains (i)

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	352/354 (99%)	343 (97%)	9 (3%)	54	79
1	B	354/354 (100%)	344 (97%)	10 (3%)	51	77
1	C	352/354 (99%)	345 (98%)	7 (2%)	63	85
1	D	352/354 (99%)	342 (97%)	10 (3%)	51	77
1	E	350/354 (99%)	336 (96%)	14 (4%)	38	63
1	F	352/354 (99%)	341 (97%)	11 (3%)	47	73
1	G	352/354 (99%)	344 (98%)	8 (2%)	58	82
1	H	352/354 (99%)	341 (97%)	11 (3%)	47	73
All	All	2816/2832 (99%)	2736 (97%)	80 (3%)	51	77

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	37	GLU
1	A	40	LEU
1	A	41	PHE
1	A	218	ARG
1	A	255	GLN
1	A	352	ASP
1	A	396	ARG
1	A	401	CYS
1	B	1	MET
1	B	37	GLU
1	B	38	ARG

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Mol	Chain	Res	Type
1	B	42	ASP
1	B	150	ASN
1	B	185	ARG
1	B	330	GLU
1	B	337	CYS
1	B	352	ASP
1	B	396	ARG
1	C	36	LEU
1	C	42	ASP
1	C	183	GLU
1	C	212	ASP
1	C	271	ARG
1	C	310	LEU
1	C	347	ARG
1	D	37	GLU
1	D	42	ASP
1	D	115	GLU
1	D	212	ASP
1	D	249	LEU
1	D	261	LYS
1	D	271	ARG
1	D	297	ASP
1	D	396	ARG
1	D	401	CYS
1	E	8	HIS
1	E	37	GLU
1	E	73	THR
1	E	109	GLU
1	E	115	GLU
1	E	185	ARG
1	E	229	LYS
1	E	256	ASN
1	E	270	ASN
1	E	304	THR
1	E	307	ASN
1	E	336	ARG
1	E	337	CYS
1	E	396	ARG
1	F	38	ARG
1	F	40	LEU
1	F	41	PHE
1	F	115	GLU

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Mol	Chain	Res	Type
1	F	185	ARG
1	F	212	ASP
1	F	270	ASN
1	F	297	ASP
1	F	352	ASP
1	F	396	ARG
1	F	401	CYS
1	G	42	ASP
1	G	72	GLU
1	G	140	GLU
1	G	141	LYS
1	G	183	GLU
1	G	185	ARG
1	G	330	GLU
1	G	401	CYS
1	H	36	LEU
1	H	38	ARG
1	H	72	GLU
1	H	185	ARG
1	H	212	ASP
1	H	249	LEU
1	H	255	GLN
1	H	336	ARG
1	H	382	LEU
1	H	396	ARG
1	H	401	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	349	GLN
1	C	179	HIS
1	C	186	ASN
1	C	270	ASN
1	C	341	ASN
1	C	349	GLN
1	D	160	ASN
1	D	291	HIS
1	D	370	ASN
1	E	199	HIS
1	E	238	GLN

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Mol	Chain	Res	Type
1	F	97	ASN
1	F	160	ASN
1	F	355	ASN
1	F	388	HIS
1	G	186	ASN
1	G	214	ASN
1	G	326	ASN
1	G	349	GLN
1	G	355	ASN
1	H	351	ASN
1	H	388	HIS

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

19 ligands are modelled in this entry.

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	SO4	A	420	-	4,4,4	1.46	0	6,6,6	0.37	0
2	SO4	A	421	-	4,4,4	0.20	0	6,6,6	0.34	0
3	PGE	A	422	-	9,9,9	0.38	0	8,8,8	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	420	-	4,4,4	1.27	0	6,6,6	0.22	0
2	SO4	B	421	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	C	420	-	4,4,4	1.79	1 (25%)	6,6,6	0.55	0
2	SO4	C	421	-	4,4,4	0.32	0	6,6,6	0.26	0
2	SO4	D	420	-	4,4,4	1.36	1 (25%)	6,6,6	0.40	0
2	SO4	D	421	-	4,4,4	0.34	0	6,6,6	0.18	0
2	SO4	E	420	-	4,4,4	0.87	0	6,6,6	0.24	0
2	SO4	E	421	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	F	420	-	4,4,4	1.60	1 (25%)	6,6,6	1.26	1 (16%)
2	SO4	F	421	-	4,4,4	0.42	0	6,6,6	0.39	0
4	PG4	F	422	-	12,12,12	0.28	0	11,11,11	0.35	0
3	PGE	F	423	-	9,9,9	0.39	0	8,8,8	0.35	0
2	SO4	G	420	-	4,4,4	1.24	0	6,6,6	0.49	0
2	SO4	G	421	-	4,4,4	0.57	0	6,6,6	0.34	0
2	SO4	H	420	-	4,4,4	1.78	1 (25%)	6,6,6	0.28	0
2	SO4	H	421	-	4,4,4	0.25	0	6,6,6	0.26	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	SO4	A	420	-	-	0/0/0/0	0/0/0/0
2	SO4	A	421	-	-	0/0/0/0	0/0/0/0
3	PGE	A	422	-	-	0/7/7/7	0/0/0/0
2	SO4	B	420	-	-	0/0/0/0	0/0/0/0
2	SO4	B	421	-	-	0/0/0/0	0/0/0/0
2	SO4	C	420	-	-	0/0/0/0	0/0/0/0
2	SO4	C	421	-	-	0/0/0/0	0/0/0/0
2	SO4	D	420	-	-	0/0/0/0	0/0/0/0
2	SO4	D	421	-	-	0/0/0/0	0/0/0/0
2	SO4	E	420	-	-	0/0/0/0	0/0/0/0
2	SO4	E	421	-	-	0/0/0/0	0/0/0/0
2	SO4	F	420	-	-	0/0/0/0	0/0/0/0
2	SO4	F	421	-	-	0/0/0/0	0/0/0/0
4	PG4	F	422	-	-	0/10/10/10	0/0/0/0
3	PGE	F	423	-	-	0/7/7/7	0/0/0/0
2	SO4	G	420	-	-	0/0/0/0	0/0/0/0
2	SO4	G	421	-	-	0/0/0/0	0/0/0/0
2	SO4	H	420	-	-	0/0/0/0	0/0/0/0
2	SO4	H	421	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	420	SO4	O3-S	-2.89	1.37	1.47
2	F	420	SO4	O2-S	-2.36	1.39	1.47
2	C	420	SO4	O3-S	-2.21	1.39	1.47
2	D	420	SO4	O1-S	-2.06	1.40	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	420	SO4	O2-S-O1	-3.03	99.90	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	420	SO4	2	0
3	A	422	PGE	20	0
2	B	420	SO4	3	0
2	C	420	SO4	3	0
2	C	421	SO4	1	0
2	D	420	SO4	2	0
2	E	420	SO4	3	0
2	F	420	SO4	4	0
4	F	422	PG4	14	0
3	F	423	PGE	4	0
2	G	420	SO4	3	0
2	H	420	SO4	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, 95^{th} 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	408/411 (99%)	0.41	14 (3%) 49 53	21, 42, 79, 114	0
1	B	411/411 (100%)	0.54	21 (5%) 32 36	29, 59, 99, 119	0
1	C	409/411 (99%)	0.39	13 (3%) 51 55	25, 45, 76, 114	0
1	D	409/411 (99%)	0.43	11 (2%) 58 61	27, 48, 79, 107	0
1	E	406/411 (98%)	1.21	80 (19%) 1 1	35, 77, 118, 146	0
1	F	409/411 (99%)	0.41	11 (2%) 58 61	22, 43, 81, 111	0
1	G	408/411 (99%)	0.75	44 (10%) 8 7	27, 59, 101, 135	0
1	H	408/411 (99%)	1.00	64 (15%) 3 2	31, 65, 116, 159	0
All	All	3268/3288 (99%)	0.64	258 (7%) 15 16	21, 54, 103, 159	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	268	ALA	9.6
1	H	253	PHE	7.1
1	H	259	PHE	6.7
1	H	301	TYR	6.5
1	C	268	ALA	6.3
1	G	253	PHE	5.7
1	E	313	VAL	5.5
1	H	310	LEU	5.5
1	E	234	VAL	5.4
1	D	144	THR	5.1
1	E	253	PHE	5.1
1	E	273	PHE	5.0
1	H	267	PHE	4.8
1	B	144	THR	4.6
1	H	250	VAL	4.6
1	B	253	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	266	GLU	4.5
1	E	225	LEU	4.5
1	E	144	THR	4.4
1	H	327	LEU	4.4
1	E	340	ASP	4.4
1	E	260	LYS	4.4
1	E	269	ASN	4.3
1	A	42	ASP	4.3
1	B	143	LEU	4.2
1	H	260	LYS	4.1
1	B	294	ILE	4.1
1	F	253	PHE	4.1
1	H	311	HIS	4.1
1	G	305	TYR	4.1
1	E	262	VAL	4.0
1	H	305	TYR	4.0
1	G	307	ASN	4.0
1	H	249	LEU	4.0
1	H	306	ASP	4.0
1	C	269	ASN	4.0
1	G	259	PHE	4.0
1	E	250	VAL	3.9
1	G	310	LEU	3.9
1	E	140	GLU	3.9
1	C	144	THR	3.8
1	H	236	ILE	3.8
1	B	269	ASN	3.8
1	H	272	LYS	3.8
1	H	175	VAL	3.8
1	H	9	VAL	3.7
1	G	258	GLY	3.7
1	A	271	ARG	3.7
1	H	300	VAL	3.7
1	B	142	GLY	3.6
1	E	306	ASP	3.6
1	E	232	LEU	3.6
1	H	296	GLY	3.6
1	E	146	LEU	3.6
1	E	83	GLU	3.6
1	A	253	PHE	3.5
1	H	269	ASN	3.5
1	E	272	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	267	PHE	3.5
1	E	256	ASN	3.5
1	E	143	LEU	3.5
1	E	355	ASN	3.4
1	E	204	GLY	3.4
1	E	7	ILE	3.4
1	E	336	ARG	3.4
1	H	298	LEU	3.4
1	B	267	PHE	3.4
1	E	171	ILE	3.4
1	H	261	LYS	3.4
1	E	115	GLU	3.4
1	E	365	VAL	3.3
1	G	311	HIS	3.3
1	C	267	PHE	3.3
1	E	305	TYR	3.3
1	E	303	VAL	3.3
1	E	332	VAL	3.3
1	H	229	LYS	3.3
1	H	313	VAL	3.3
1	B	271	ARG	3.3
1	D	143	LEU	3.3
1	H	322	LEU	3.2
1	E	214	ASN	3.2
1	B	293	GLU	3.2
1	E	263	LEU	3.2
1	E	136	ILE	3.2
1	G	210	VAL	3.2
1	E	268	ALA	3.2
1	E	142	GLY	3.2
1	G	298	LEU	3.2
1	G	233	ALA	3.2
1	E	231	VAL	3.1
1	E	114	ILE	3.1
1	E	295	GLU	3.1
1	H	209	MET	3.1
1	G	262	VAL	3.1
1	E	226	VAL	3.1
1	G	231	VAL	3.1
1	E	329	VAL	3.1
1	H	263	LEU	3.0
1	H	319	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	259	PHE	3.0
1	E	323	LEU	3.0
1	D	4	GLN	3.0
1	G	236	ILE	3.0
1	H	299	ARG	3.0
1	G	249	LEU	3.0
1	H	307	ASN	3.0
1	H	411	ILE	2.9
1	A	273	PHE	2.9
1	H	252	ILE	2.9
1	G	272	LYS	2.9
1	D	269	ASN	2.9
1	F	3	ALA	2.9
1	H	248	LEU	2.9
1	H	302	SER	2.9
1	F	273	PHE	2.9
1	G	252	ILE	2.9
1	A	40	LEU	2.8
1	E	177	LEU	2.8
1	E	267	PHE	2.8
1	D	294	ILE	2.8
1	C	143	LEU	2.8
1	C	146	LEU	2.8
1	G	209	MET	2.8
1	E	319	LEU	2.8
1	B	140	GLU	2.8
1	C	136	ILE	2.7
1	E	294	ILE	2.7
1	F	136	ILE	2.7
1	G	313	VAL	2.7
1	E	359	ILE	2.7
1	D	136	ILE	2.7
1	E	183	GLU	2.7
1	H	210	VAL	2.7
1	G	301	TYR	2.7
1	B	225	LEU	2.7
1	E	216	THR	2.7
1	A	267	PHE	2.7
1	E	261	LYS	2.7
1	E	175	VAL	2.7
1	H	231	VAL	2.7
1	G	297	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	252	ILE	2.6
1	E	274	MET	2.6
1	F	254	LYS	2.6
1	E	236	ILE	2.6
1	H	181	PHE	2.6
1	E	210	VAL	2.6
1	B	146	LEU	2.6
1	G	269	ASN	2.6
1	H	144	THR	2.6
1	E	312	ILE	2.5
1	F	43	ASP	2.5
1	D	270	ASN	2.5
1	E	292	PRO	2.5
1	B	249	LEU	2.5
1	B	305	TYR	2.5
1	E	248	LEU	2.5
1	F	294	ILE	2.5
1	E	298	LEU	2.5
1	H	146	LEU	2.5
1	E	293	GLU	2.5
1	A	297	ASP	2.5
1	E	310	LEU	2.5
1	E	235	GLY	2.5
1	A	43	ASP	2.4
1	A	306	ASP	2.4
1	E	86	GLU	2.4
1	H	308	GLU	2.4
1	A	274	MET	2.4
1	H	273	PHE	2.4
1	H	204	GLY	2.4
1	G	13	ILE	2.4
1	G	290	ILE	2.4
1	G	242	ALA	2.4
1	H	246	GLU	2.4
1	G	254	LYS	2.4
1	A	268	ALA	2.4
1	B	340	ASP	2.4
1	E	102	ALA	2.4
1	H	171	ILE	2.4
1	E	265	PHE	2.4
1	H	214	ASN	2.4
1	B	40	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	312	ILE	2.4
1	G	411	ILE	2.4
1	G	306	ASP	2.3
1	E	79	LEU	2.3
1	D	411	ILE	2.3
1	B	214	ASN	2.3
1	E	101	ARG	2.3
1	F	39	LEU	2.3
1	G	175	VAL	2.3
1	H	256	ASN	2.3
1	G	181	PHE	2.3
1	G	9	VAL	2.3
1	H	303	VAL	2.3
1	H	295	GLU	2.3
1	C	273	PHE	2.3
1	G	177	LEU	2.3
1	E	215	GLU	2.3
1	E	275	HIS	2.3
1	H	251	ASN	2.3
1	C	137	PRO	2.3
1	G	7	ILE	2.3
1	D	273	PHE	2.3
1	C	184	THR	2.3
1	G	230	ASP	2.3
1	E	337	CYS	2.2
1	G	296	GLY	2.2
1	E	9	VAL	2.2
1	E	194	TYR	2.2
1	H	316	LYS	2.2
1	F	37	GLU	2.2
1	H	257	LEU	2.2
1	F	297	ASP	2.2
1	H	242	ALA	2.2
1	E	296	GLY	2.2
1	E	109	GLU	2.2
1	G	250	VAL	2.2
1	H	201	ILE	2.2
1	B	295	GLU	2.2
1	D	267	PHE	2.2
1	H	5	THR	2.2
1	H	228	SER	2.1
1	H	258	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	411	ILE	2.1
1	B	257	LEU	2.1
1	G	303	VAL	2.1
1	E	249	LEU	2.1
1	H	276	LEU	2.1
1	E	198	HIS	2.1
1	H	208	PRO	2.1
1	G	336	ARG	2.1
1	C	133	LEU	2.1
1	G	276	LEU	2.1
1	H	41	PHE	2.1
1	G	299	ARG	2.1
1	G	268	ALA	2.1
1	A	411	ILE	2.1
1	G	10	TYR	2.1
1	H	136	ILE	2.1
1	B	83	GLU	2.1
1	B	352	ASP	2.1
1	A	28	ILE	2.1
1	F	236	ILE	2.1
1	H	172	GLY	2.1
1	G	263	LEU	2.1
1	E	352	ASP	2.1
1	A	298	LEU	2.0
1	H	196	PHE	2.0
1	H	403	SER	2.0
1	C	99	ARG	2.0
1	E	271	ARG	2.0
1	E	154	ALA	2.0
1	H	268	ALA	2.0
1	C	271	ARG	2.0
1	E	288	PHE	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

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, 95^{th} 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	SO4	D	420	5/5	0.92	0.35	12.90	26,30,34,36	5
3	PGE	A	422	10/10	0.88	0.37	9.60	35,41,43,44	0
2	SO4	E	420	5/5	0.95	0.43	9.48	34,37,39,43	5
2	SO4	B	420	5/5	0.96	0.41	7.64	30,30,34,37	5
2	SO4	A	420	5/5	0.96	0.31	5.77	16,19,20,24	5
2	SO4	C	420	5/5	0.93	0.28	5.59	21,26,30,34	5
2	SO4	G	420	5/5	0.96	0.31	4.09	25,26,33,35	5
2	SO4	H	420	5/5	0.97	0.24	2.65	26,29,36,37	5
3	PGE	F	423	10/10	0.81	0.29	2.26	49,60,66,67	0
2	SO4	H	421	5/5	0.82	0.35	2.19	94,95,96,96	5
4	PG4	F	422	13/13	0.82	0.29	1.74	59,62,67,68	0
2	SO4	F	420	5/5	0.99	0.22	1.25	18,20,22,23	5
2	SO4	D	421	5/5	0.88	0.28	0.42	79,80,80,80	5
2	SO4	C	421	5/5	0.96	0.22	-0.13	57,58,60,60	5
2	SO4	G	421	5/5	0.94	0.19	-0.18	52,54,57,58	5
2	SO4	F	421	5/5	0.97	0.16	-0.50	55,56,57,62	0
2	SO4	A	421	5/5	0.98	0.16	-0.99	46,51,52,54	0
2	SO4	B	421	5/5	0.93	0.19	-1.14	91,91,91,91	5
2	SO4	E	421	5/5	0.89	0.16	-2.17	101,101,102,102	5

6.5 Other polymers

There are no such residues in this entry.