Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:44 PM GMT

PDB ID	:	4ACB
Title	:	CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR SELB FROM METHANOCOCCUS MARIPALUDIS IN COMPLEX WITH THE GTP ANALOGUE GPPNHP
Authors	:	Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on	:	2011-12-14
Resolution	:	3.34 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

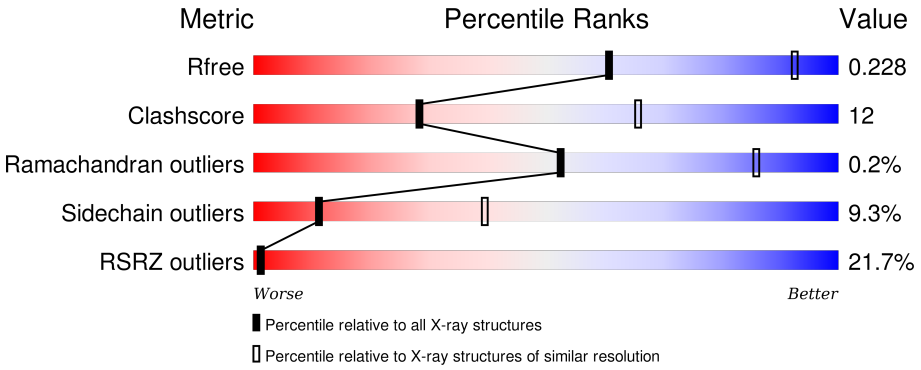
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.34 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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	482	21% 67% 24% • 6%
1	B	482	15% 65% 26% • 5%
1	C	482	4% 67% 27% • •
1	D	482	42% 67% 25% 5% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CMH	D	340	-	-	X	-
5	SO4	B	1472	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14623 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 TRANSLATION ELONGATION FACTOR SELB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	Hg	N	O	S	0	0	0
			3506	2240	4	597	651	14			
1	B	456	Total	C	Hg	N	O	S	0	0	0
			3533	2257	4	603	655	14			
1	C	471	Total	C	Hg	N	O	S	0	0	0
			3651	2327	4	627	679	14			
1	D	467	Total	C	Hg	N	O	S	0	0	0
			3615	2305	4	618	675	13			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q8J307
A	-12	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-11	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-10	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-9	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-8	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-7	HIS	-	EXPRESSION TAG	UNP Q8J307
A	-6	SER	-	EXPRESSION TAG	UNP Q8J307
A	-5	ILE	-	EXPRESSION TAG	UNP Q8J307
A	-4	GLU	-	EXPRESSION TAG	UNP Q8J307
A	-3	GLY	-	EXPRESSION TAG	UNP Q8J307
A	-2	ARG	-	EXPRESSION TAG	UNP Q8J307
A	-1	PRO	-	EXPRESSION TAG	UNP Q8J307
A	0	HIS	-	EXPRESSION TAG	UNP Q8J307
B	-13	MET	-	EXPRESSION TAG	UNP Q8J307
B	-12	HIS	-	EXPRESSION TAG	UNP Q8J307
B	-11	HIS	-	EXPRESSION TAG	UNP Q8J307
B	-10	HIS	-	EXPRESSION TAG	UNP Q8J307
B	-9	HIS	-	EXPRESSION TAG	UNP Q8J307
B	-8	HIS	-	EXPRESSION TAG	UNP Q8J307
B	-7	HIS	-	EXPRESSION TAG	UNP Q8J307

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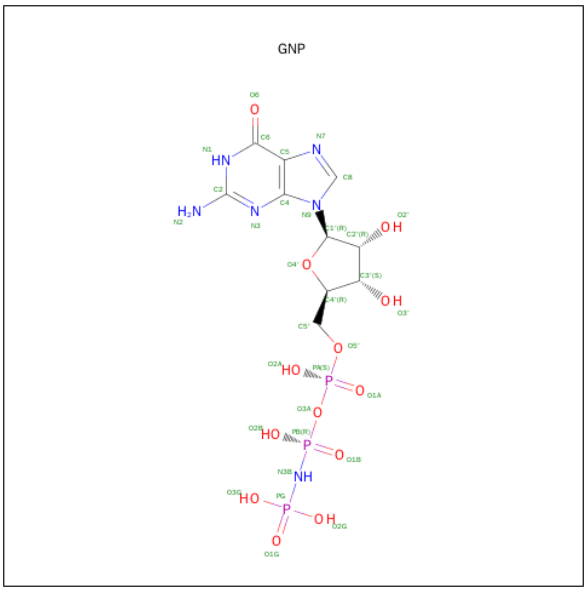
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	EXPRESSION TAG	UNP Q8J307
B	-5	ILE	-	EXPRESSION TAG	UNP Q8J307
B	-4	GLU	-	EXPRESSION TAG	UNP Q8J307
B	-3	GLY	-	EXPRESSION TAG	UNP Q8J307
B	-2	ARG	-	EXPRESSION TAG	UNP Q8J307
B	-1	PRO	-	EXPRESSION TAG	UNP Q8J307
B	0	HIS	-	EXPRESSION TAG	UNP Q8J307
C	-13	MET	-	EXPRESSION TAG	UNP Q8J307
C	-12	HIS	-	EXPRESSION TAG	UNP Q8J307
C	-11	HIS	-	EXPRESSION TAG	UNP Q8J307
C	-10	HIS	-	EXPRESSION TAG	UNP Q8J307
C	-9	HIS	-	EXPRESSION TAG	UNP Q8J307
C	-8	HIS	-	EXPRESSION TAG	UNP Q8J307
C	-7	HIS	-	EXPRESSION TAG	UNP Q8J307
C	-6	SER	-	EXPRESSION TAG	UNP Q8J307
C	-5	ILE	-	EXPRESSION TAG	UNP Q8J307
C	-4	GLU	-	EXPRESSION TAG	UNP Q8J307
C	-3	GLY	-	EXPRESSION TAG	UNP Q8J307
C	-2	ARG	-	EXPRESSION TAG	UNP Q8J307
C	-1	PRO	-	EXPRESSION TAG	UNP Q8J307
C	0	HIS	-	EXPRESSION TAG	UNP Q8J307
D	-13	MET	-	EXPRESSION TAG	UNP Q8J307
D	-12	HIS	-	EXPRESSION TAG	UNP Q8J307
D	-11	HIS	-	EXPRESSION TAG	UNP Q8J307
D	-10	HIS	-	EXPRESSION TAG	UNP Q8J307
D	-9	HIS	-	EXPRESSION TAG	UNP Q8J307
D	-8	HIS	-	EXPRESSION TAG	UNP Q8J307
D	-7	HIS	-	EXPRESSION TAG	UNP Q8J307
D	-6	SER	-	EXPRESSION TAG	UNP Q8J307
D	-5	ILE	-	EXPRESSION TAG	UNP Q8J307
D	-4	GLU	-	EXPRESSION TAG	UNP Q8J307
D	-3	GLY	-	EXPRESSION TAG	UNP Q8J307
D	-2	ARG	-	EXPRESSION TAG	UNP Q8J307
D	-1	PRO	-	EXPRESSION TAG	UNP Q8J307
D	0	HIS	-	EXPRESSION TAG	UNP Q8J307

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

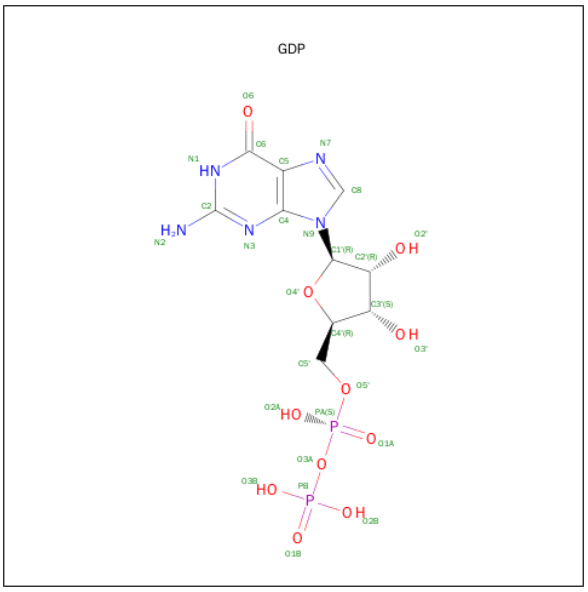


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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

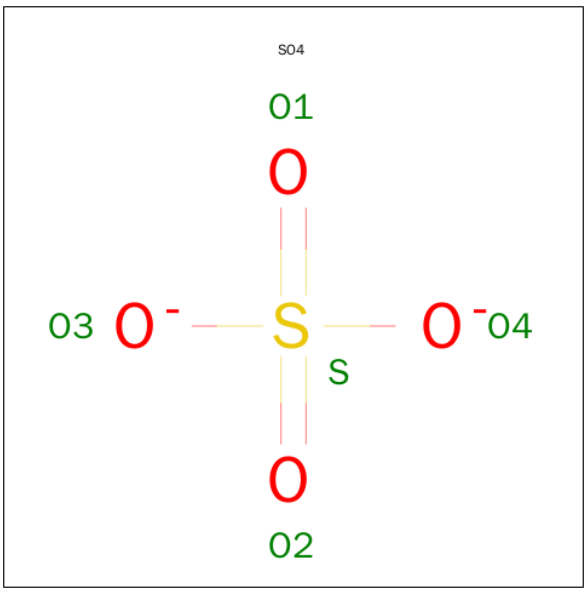
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	O	S		0	0
			5	4	1			
5	B	1	Total	O	S		0	0
			5	4	1			
5	C	1	Total	O	S		0	0
			5	4	1			

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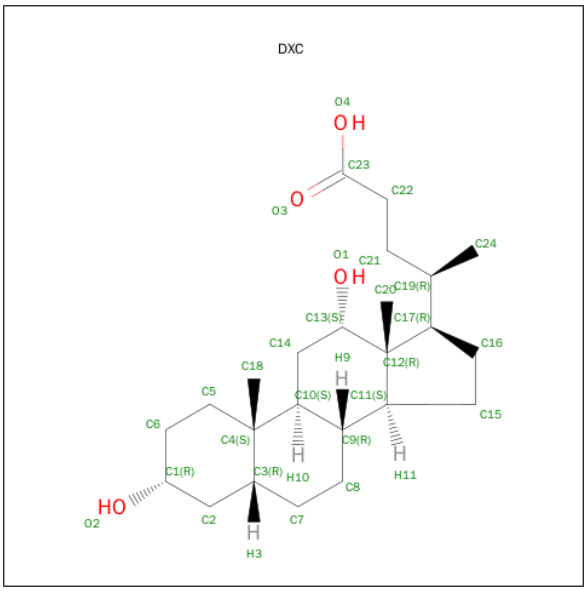
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

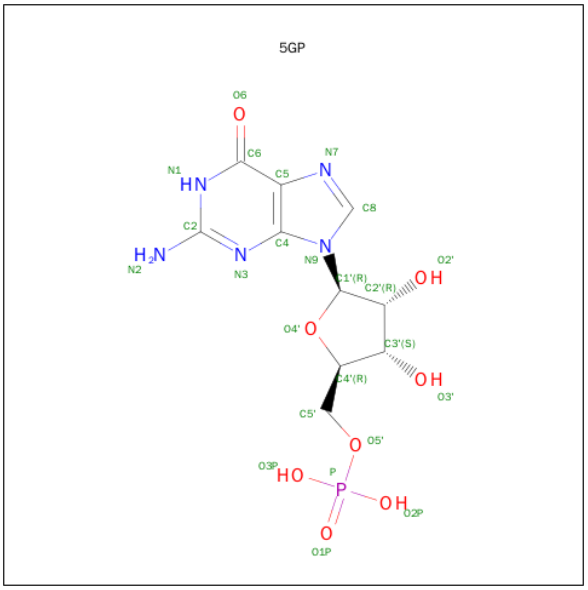
- Molecule 6 is (3ALPHA,5BETA,12ALPHA)-3,12-DIHYDROXYCHOLAN-24-OIC ACID (three-letter code: DXC) (formula: $C_{24}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 28 24 4	0	0
6	C	1	Total C O 28 24 4	0	0
6	C	1	Total C O 28 24 4	0	0
6	C	1	Total C O 28 24 4	0	0
6	C	1	Total C O 28 24 4	0	0
6	C	1	Total C O 28 24 4	0	0
6	C	1	Total C O 28 24 4	0	0

- Molecule 7 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:

$C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 8 is water.

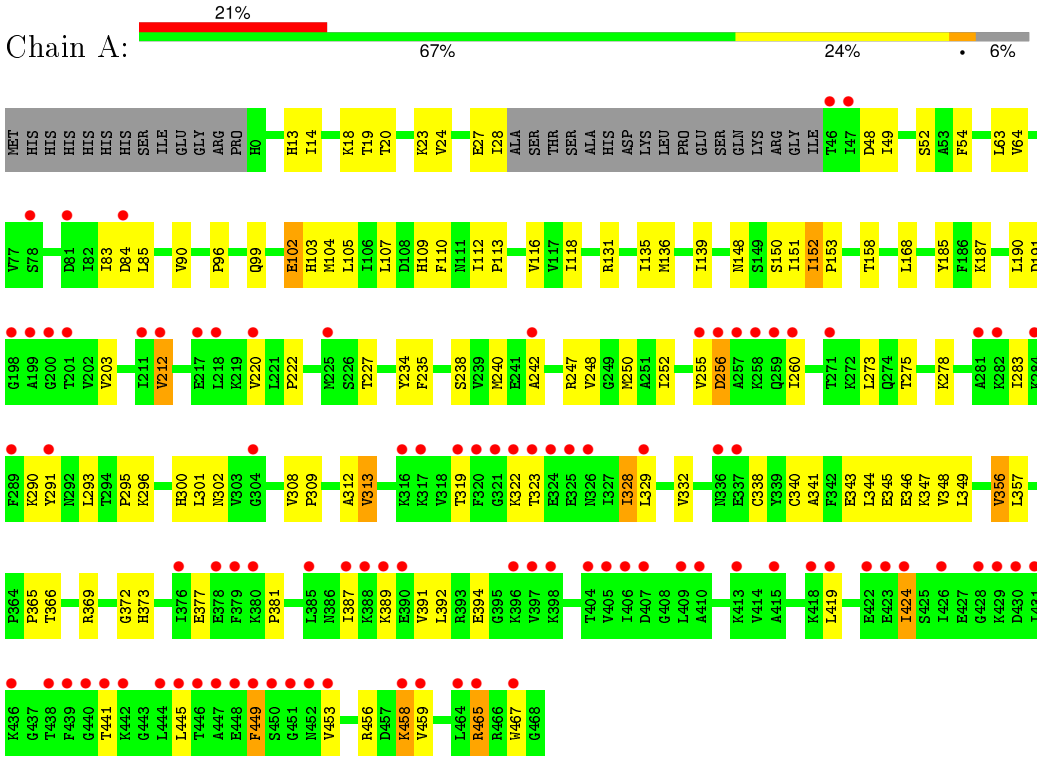
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	O	0	0
			2	2		
8	B	4	Total	O	0	0
			4	4		

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.

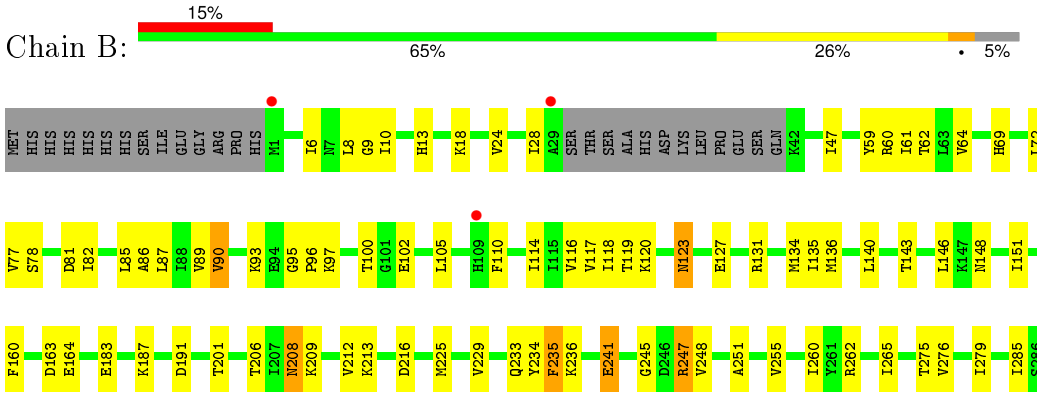
- Molecule 1: TRANSLATION ELONGATION FACTOR SELB

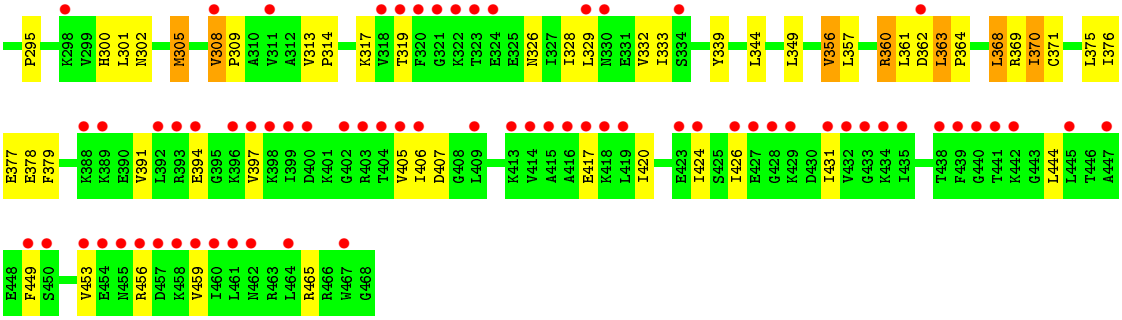
Chain A:



- Molecule 1: TRANSLATION ELONGATION FACTOR SELB

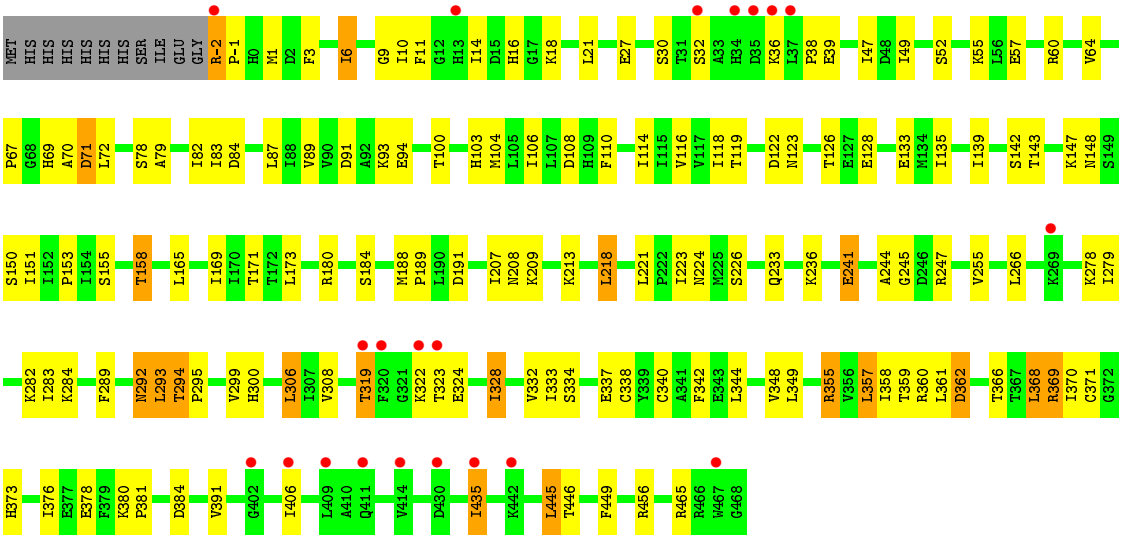
Chain B:





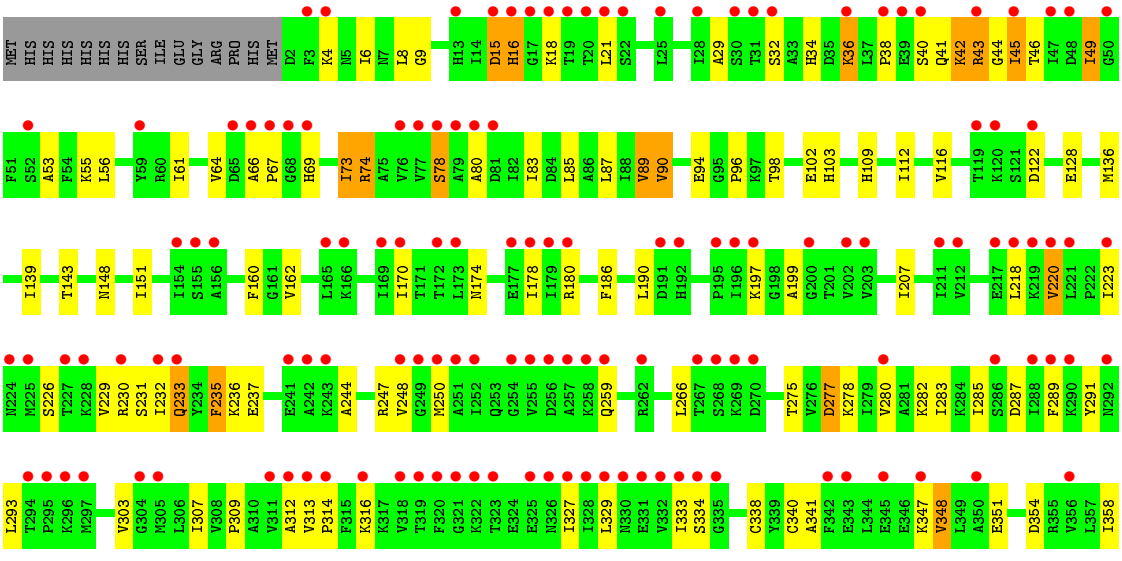
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

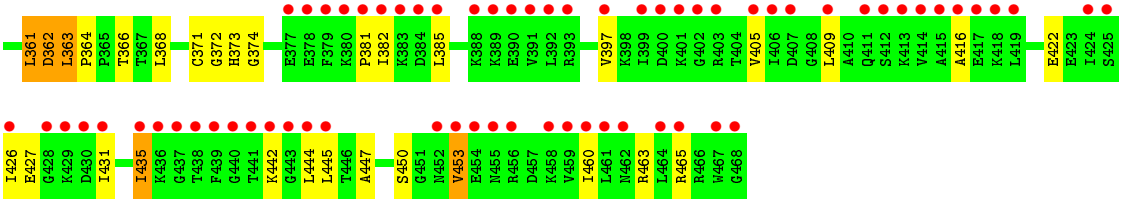
Chain C:



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

Chain D:




L361
D362
L363
P364
P365
T366
T367
L368
C371
G372
H373
G374
E377
E378
F379
K380
P381
I382
K383
D384
L385
K388
K389
E390
V391
L392
R393
V397
K398
I399
D400
K401
G402
R403
T404
V405
I406
D407
G408
L409
A410
Q411
S412
K413
V414
A415
A416
E417
K418
L419
E422
E423
I424
S425
I426
E427
G428
K429
D430
I431
I435
K436
G437
T438
F439
G440
T441
K442
G443
L444
L445
T446
A447
S450
G451
N452
V453
E454
N455
R456
D457
K458
V459
I460
L461
N462
R463
L464
R465
R466
W467
G468

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	146.63Å 146.63Å 297.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.34 34.48 – 3.34	Depositor EDS
% Data completeness (in resolution range)	82.8 (19.94-3.34) 88.5 (34.48-3.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.179 , 0.223 0.195 , 0.228	Depositor DCC
R_{free} test set	2204 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	110.2	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 153.3	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 53119 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14623	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: GDP, GNP, CMH, MG, SO4, 5GP, DXC

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	0.31	0/3515	0.55	0/4727
1	B	0.35	0/3541	0.57	0/4760
1	C	0.40	0/3664	0.63	0/4929
1	D	0.28	0/3626	0.53	0/4878
All	All	0.34	0/14346	0.57	0/19294

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

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	3506	0	3687	73	0
1	B	3533	0	3726	84	0
1	C	3651	0	3838	82	0
1	D	3615	0	3801	107	0
2	A	32	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	28	0	12	2	0
5	B	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	20	0	0	2	0
6	B	28	0	39	4	0
6	C	168	0	234	15	0
7	B	24	0	12	2	0
8	A	2	0	0	0	0
8	B	4	0	0	0	0
All	All	14623	0	15362	349	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 12.

All (349) 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:6:ILE:HD12	1:C:173:LEU:HD13	1.54	0.90
1:C:338:CMH:HB3	1:C:340:CMH:CM	2.05	0.86
1:D:43:ARG:HD3	1:D:45:ILE:HD11	1.57	0.85
1:D:283:ILE:HG13	1:D:340:CMH:HB3	1.61	0.82
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.61	0.80
1:C:27:GLU:HB3	1:C:32:SER:HB2	1.63	0.79
1:C:306:LEU:HD13	1:C:348:VAL:HG22	1.65	0.79
1:D:45:ILE:HB	1:D:233:GLN:HE22	1.47	0.78
1:D:416:ALA:HB1	1:D:445:LEU:HD21	1.65	0.77
1:A:234:TYR:HB2	1:A:248:VAL:HG12	1.68	0.76
1:A:116:VAL:HB	1:A:151:ILE:HG12	1.68	0.75
1:D:43:ARG:HB3	1:D:45:ILE:HG13	1.67	0.75
1:C:283:ILE:HD13	1:C:340:CMH:HB3	1.70	0.73
1:B:251:ALA:HB1	1:C:1:MET:HE1	1.70	0.73
1:D:67:PRO:HA	1:D:78:SER:HB2	1.71	0.72
1:B:361:LEU:HD23	1:B:369:ARG:HD2	1.71	0.72
1:A:54:PHE:HE1	1:A:63:LEU:HD13	1.57	0.70
1:A:240:MET:HE1	1:B:95:GLY:HA3	1.73	0.69
1:C:368:LEU:HD12	1:C:370:ILE:H	1.56	0.69
1:D:293:LEU:HD21	1:D:340:CMH:CM	2.23	0.68
1:A:99:GLN:NE2	1:A:102:GLU:OE2	2.27	0.67
1:D:74:ARG:HH22	1:D:309:PRO:HD3	1.57	0.67
1:A:435:ILE:HD11	1:A:445:LEU:HD22	1.75	0.66
1:D:427:GLU:HG2	1:D:460:ILE:HG13	1.78	0.66
1:C:289:PHE:CE2	1:C:371:CMH:HB2	2.31	0.66
1:A:152:ILE:HD11	1:A:168:LEU:HD22	1.77	0.65
1:D:313:VAL:HB	1:D:341:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASP:N	1:A:362:ASP:OD1	2.28	0.64
1:B:158:THR:HG23	1:D:363:LEU:HB3	1.80	0.64
1:B:302:ASN:HB2	1:B:357:LEU:HB3	1.79	0.64
1:D:45:ILE:HB	1:D:233:GLN:NE2	2.12	0.63
1:C:308:VAL:HG21	1:C:344:LEU:HD13	1.80	0.63
1:A:433:GLY:HA3	1:A:449:PHE:HB3	1.80	0.63
1:D:422:GLU:H	1:D:435:ILE:HG22	1.63	0.63
1:D:338:CMH:CM	1:D:340:CMH:SG	2.87	0.63
1:B:191:ASP:OD2	1:B:247:ARG:NH1	2.25	0.62
1:D:409:LEU:HD12	1:D:445:LEU:HD12	1.81	0.62
1:B:363:LEU:HD13	1:B:364:PRO:HD2	1.82	0.62
1:A:70:ALA:O	1:A:369:ARG:NH2	2.32	0.62
1:C:293:LEU:HD22	1:C:371:CMH:CM	2.30	0.62
1:D:36:LYS:HB3	1:D:236:LYS:HD2	1.81	0.61
1:C:100:THR:O	1:C:104:MET:HG3	2.01	0.61
1:A:278:LYS:HD2	1:A:343:GLU:HG2	1.82	0.60
1:D:74:ARG:HG2	1:D:361:LEU:HD13	1.82	0.60
1:C:283:ILE:HG12	1:C:358:ILE:HD11	1.82	0.60
1:A:313:VAL:HG23	1:A:341:ALA:HB3	1.82	0.60
1:D:435:ILE:HG13	1:D:447:ALA:HB2	1.83	0.60
1:C:435:ILE:HD12	1:C:445:LEU:HD13	1.83	0.59
1:B:10:ILE:HD13	1:B:87:LEU:HB2	1.84	0.59
1:B:216:ASP:O	1:B:229:VAL:HG23	2.02	0.59
1:B:287:ASP:OD1	1:B:287:ASP:N	2.28	0.59
1:B:187:LYS:HB3	1:B:209:LYS:HG3	1.84	0.59
1:B:233:GLN:HE21	1:B:236:LYS:HA	1.67	0.59
1:D:316:LYS:N	1:D:327:ILE:O	2.35	0.58
1:B:90:VAL:HG13	1:B:118:ILE:HG12	1.84	0.58
1:A:222:PRO:HB3	1:A:349:LEU:HD21	1.85	0.58
1:D:43:ARG:HD3	1:D:45:ILE:CD1	2.33	0.58
1:B:288:ILE:HB	7:B:1474:5GP:HN22	1.68	0.58
1:A:312:ALA:HB1	1:A:340:CMH:SG	2.42	0.58
1:D:314:PRO:HB3	1:D:338:CMH:CM	2.34	0.57
1:A:18:LYS:NZ	2:A:1469:GNP:O1B	2.33	0.57
1:C:381:PRO:HD2	1:C:384:ASP:HB2	1.84	0.57
1:A:295:PRO:HG3	1:A:328:ILE:HD11	1.84	0.57
1:A:391:VAL:HG21	1:A:465:ARG:HD3	1.86	0.57
1:D:116:VAL:HG11	1:D:136:MET:HG2	1.86	0.57
1:C:10:ILE:HG22	1:C:18:LYS:HG3	1.87	0.57
1:B:233:GLN:OE1	6:B:1473:DXC:H10	2.05	0.56
1:A:308:VAL:HG21	1:A:344:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HG23	1:A:467:TRP:HB3	1.87	0.56
1:A:76:VAL:HG11	1:A:103:HIS:CD2	2.41	0.56
1:C:295:PRO:HG2	1:C:328:ILE:HD11	1.88	0.56
1:D:8:LEU:HD11	1:D:87:LEU:HG	1.87	0.55
1:A:256:ASP:OD1	1:A:256:ASP:N	2.30	0.55
1:D:232:ILE:HG12	1:D:250:MET:HG2	1.87	0.55
1:C:36:LYS:HE3	1:C:38:PRO:HB3	1.87	0.55
1:C:69:HIS:CD2	1:C:70:ALA:H	2.24	0.55
1:B:301:LEU:HD11	1:B:356:VAL:HG13	1.88	0.55
1:D:397:VAL:HG11	1:D:453:VAL:HB	1.88	0.55
1:A:238:SER:H	1:B:97:LYS:NZ	2.05	0.55
1:B:74:ARG:NH2	5:B:1471:SO4:O4	2.40	0.55
1:D:15:ASP:HA	1:D:18:LYS:HE2	1.89	0.54
1:B:9:GLY:HA2	1:B:64:VAL:HB	1.88	0.54
5:B:1472:SO4:O2	1:C:55:LYS:NZ	2.41	0.54
1:A:300:HIS:CE1	1:A:309:PRO:HG3	2.42	0.54
1:B:116:VAL:HB	1:B:151:ILE:HG12	1.90	0.54
1:A:96:PRO:HB3	1:A:136:MET:HE3	1.90	0.54
1:D:313:VAL:O	1:D:341:ALA:N	2.41	0.54
1:C:16:HIS:NE2	1:C:94:GLU:OE2	2.42	0.53
1:B:78:SER:HB2	1:B:305:MET:HG2	1.89	0.53
1:D:74:ARG:HH11	1:D:307:ILE:HG22	1.73	0.53
1:B:69:HIS:NE2	1:B:102:GLU:OE1	2.26	0.53
1:B:13:HIS:H	1:B:100:THR:HG22	1.74	0.53
1:B:426:ILE:HB	1:B:431:ILE:HG23	1.91	0.53
1:D:285:ILE:HD11	1:D:291:TYR:HB2	1.90	0.53
1:D:90:VAL:HG11	1:D:136:MET:HE1	1.91	0.53
1:D:303:VAL:HB	1:D:348:VAL:HG11	1.91	0.53
1:A:285:ILE:HG12	1:A:291:TYR:CE2	2.44	0.53
1:B:82:ILE:HD13	1:B:206:THR:HG22	1.90	0.53
1:D:180:ARG:HB3	1:D:244:ALA:HB3	1.91	0.52
1:D:34:HIS:N	1:D:53:ALA:O	2.42	0.52
1:B:314:PRO:HA	1:B:339:TYR:O	2.10	0.52
1:C:279:ILE:HD13	1:C:376:ILE:HD11	1.89	0.52
1:B:391:VAL:HB	1:B:465:ARG:HD3	1.92	0.52
1:D:277:ASP:HB3	1:D:347:LYS:HE2	1.91	0.52
1:C:1:MET:HE3	6:C:1476:DXC:H52	1.91	0.52
1:A:13:HIS:ND1	1:A:99:GLN:HG2	2.24	0.52
1:D:218:LEU:HD11	1:D:229:VAL:HG22	1.90	0.52
1:D:287:ASP:HB2	1:D:291:TYR:HE1	1.75	0.52
1:B:251:ALA:HB1	1:C:1:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD12	1:C:21:LEU:HD23	1.92	0.52
1:C:322:LYS:HG3	1:C:323:THR:H	1.75	0.52
1:C:91:ASP:HB3	1:C:94:GLU:HG2	1.90	0.52
1:D:316:LYS:HB2	1:D:329:LEU:HD13	1.92	0.51
1:C:11:PHE:CE1	1:C:72:LEU:HD22	2.44	0.51
1:D:43:ARG:HH11	1:D:231:SER:HB3	1.74	0.51
1:D:283:ILE:HA	1:D:373:HIS:O	2.11	0.51
1:A:109:HIS:HD2	1:A:373:HIS:HB3	1.76	0.51
1:D:21:LEU:HD22	1:D:89:VAL:HG11	1.92	0.51
1:B:201:THR:OG1	1:B:255:VAL:O	2.18	0.51
1:A:191:ASP:OD2	1:A:247:ARG:NH2	2.43	0.51
1:D:382:ILE:HA	1:D:385:LEU:HD12	1.92	0.51
1:C:27:GLU:HA	1:C:30:SER:HB3	1.93	0.51
1:C:82:ILE:HG23	1:C:245:GLY:HA2	1.92	0.51
1:A:360:ARG:HG2	1:A:363:LEU:HG	1.93	0.50
1:B:6:ILE:HG22	1:B:61:ILE:HG23	1.92	0.50
1:C:49:ILE:HD11	6:C:1475:DXC:H161	1.94	0.50
1:D:4:LYS:NZ	1:D:178:ILE:O	2.44	0.50
1:B:13:HIS:CE1	1:B:97:LYS:HG3	2.47	0.50
1:C:110:PHE:CD1	1:C:355:ARG:HD2	2.47	0.50
1:D:29:ALA:HB2	1:D:56:LEU:HG	1.93	0.50
1:D:40:SER:O	1:D:44:GLY:HA2	2.12	0.50
1:D:69:HIS:CE1	1:D:103:HIS:CE1	2.99	0.50
1:B:81:ASP:OD2	1:B:208:ASN:ND2	2.45	0.50
1:A:389:LYS:HB3	1:A:465:ARG:HB3	1.94	0.50
1:D:218:LEU:HD13	1:D:266:LEU:HD11	1.94	0.50
1:D:282:LYS:O	1:D:374:GLY:HA3	2.12	0.50
1:B:160:PHE:CZ	1:D:98:THR:HG23	2.47	0.50
1:D:122:ASP:N	1:D:122:ASP:OD1	2.45	0.50
1:B:72:LEU:O	1:B:76:VAL:HG23	2.12	0.50
1:C:342:PHE:HZ	1:C:358:ILE:HD13	1.75	0.49
1:D:43:ARG:HH12	1:D:230:ARG:HB3	1.76	0.49
1:D:66:ALA:HB1	1:D:69:HIS:ND1	2.26	0.49
1:B:8:LEU:HD12	1:B:85:LEU:O	2.12	0.49
1:D:38:PRO:HB3	1:D:42:LYS:HD2	1.94	0.49
1:B:233:GLN:OE1	6:B:1473:DXC:H61	2.13	0.49
1:A:238:SER:H	1:B:97:LYS:HZ3	1.58	0.49
1:C:11:PHE:HB3	1:C:103:HIS:ND1	2.27	0.49
1:D:42:LYS:HE2	1:D:237:GLU:HA	1.95	0.49
1:A:275:THR:HG22	1:A:347:LYS:HD2	1.95	0.49
1:D:358:ILE:HG22	1:D:371:CMH:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG21	1:A:64:VAL:HG13	1.94	0.49
1:A:110:PHE:CZ	1:A:357:LEU:HD13	2.47	0.49
1:A:424:ILE:HG13	1:A:459:VAL:HG13	1.95	0.48
1:D:15:ASP:OD1	1:D:16:HIS:ND1	2.46	0.48
1:A:48:ASP:OD1	1:A:49:ILE:N	2.41	0.48
1:C:122:ASP:OD2	1:C:155:SER:OG	2.29	0.48
1:B:317:LYS:HG2	1:B:326:ASN:OD1	2.14	0.48
1:D:73:ILE:O	1:D:74:ARG:HG3	2.13	0.48
1:B:82:ILE:HG23	1:B:245:GLY:HA2	1.96	0.48
1:B:329:LEU:HB3	1:B:332:VAL:HB	1.95	0.48
1:B:265:ILE:HG13	1:B:349:LEU:HD12	1.95	0.48
1:D:277:ASP:HB3	1:D:347:LYS:HG2	1.95	0.48
1:B:102:GLU:HG2	1:B:368:LEU:HD23	1.95	0.48
1:D:83:ILE:HG22	1:D:112:ILE:HD13	1.95	0.48
1:D:405:VAL:CG1	1:D:444:LEU:HB3	2.44	0.47
1:D:248:VAL:HG12	1:D:250:MET:HG3	1.96	0.47
1:A:23:LYS:O	1:A:27:GLU:HG2	2.14	0.47
1:B:406:ILE:HD11	1:B:449:PHE:HZ	1.80	0.47
1:C:213:LYS:HE2	1:C:241:GLU:OE1	2.14	0.47
1:D:431:ILE:HB	1:D:450:SER:O	2.14	0.47
1:B:93:LYS:HE3	1:B:123:ASN:O	2.14	0.47
1:D:280:VAL:HG21	1:D:385:LEU:HD21	1.97	0.47
1:C:233:GLN:OE1	6:C:1475:DXC:H11	2.14	0.47
1:A:290:LYS:HA	1:A:290:LYS:HD3	1.73	0.47
1:B:86:ALA:HB3	1:B:114:ILE:HG22	1.97	0.47
1:A:105:LEU:O	1:A:109:HIS:ND1	2.44	0.47
1:B:377:GLU:HG2	1:B:378:GLU:HG3	1.97	0.47
1:B:208:ASN:HB3	1:B:209:LYS:HG2	1.96	0.47
1:C:106:ILE:HG12	1:C:357:LEU:HD21	1.97	0.47
1:D:278:LYS:HD3	1:D:381:PRO:HA	1.97	0.47
1:B:362:ASP:OD1	1:B:363:LEU:N	2.48	0.46
1:B:120:LYS:HD3	4:B:1469:GDP:C4	2.50	0.46
1:B:291:TYR:HD1	1:B:333:ILE:HG22	1.79	0.46
1:D:197:LYS:HB3	1:D:199:ALA:H	1.79	0.46
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.81	0.46
1:D:102:GLU:HB2	1:D:366:THR:HG22	1.97	0.46
1:B:105:LEU:HD12	1:B:368:LEU:HD22	1.97	0.46
1:C:233:GLN:HE21	1:C:236:LYS:HA	1.81	0.46
1:A:227:THR:HG21	1:A:255:VAL:HG22	1.96	0.46
1:B:213:LYS:HG2	1:B:241:GLU:HB2	1.97	0.46
1:B:234:TYR:HB2	1:B:248:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:MET:HE2	1:C:104:MET:HB3	1.80	0.46
1:A:283:ILE:HD12	1:A:340:CMH:HB3	1.98	0.46
1:D:69:HIS:CE1	1:D:103:HIS:NE2	2.84	0.46
1:C:133:GLU:HG3	1:C:151:ILE:HG21	1.98	0.46
1:A:20:THR:O	1:A:24:VAL:HG23	2.15	0.46
1:D:116:VAL:HB	1:D:151:ILE:HG12	1.96	0.46
1:D:358:ILE:HB	1:D:372:GLY:N	2.31	0.46
1:D:109:HIS:HB3	1:D:373:HIS:CE1	2.51	0.46
1:C:289:PHE:CD2	1:C:371:CMH:HB2	2.51	0.46
1:A:107:LEU:HD23	1:A:112:ILE:HD12	1.96	0.46
1:C:282:LYS:HE2	1:C:337:GLU:HG2	1.97	0.46
1:C:333:ILE:HD12	6:C:1480:DXC:H203	1.98	0.46
1:C:158:THR:HG21	6:C:1478:DXC:O2	2.15	0.46
6:B:1473:DXC:H10	6:B:1473:DXC:H61	1.60	0.45
1:C:10:ILE:O	1:C:18:LYS:HE3	2.16	0.45
1:B:155:SER:HB3	1:B:160:PHE:HB3	1.99	0.45
1:C:93:LYS:HG3	1:C:128:GLU:OE1	2.16	0.45
1:A:456:ARG:O	1:A:458:LYS:NZ	2.35	0.45
1:A:283:ILE:HB	1:A:338:CMH:O	2.17	0.45
1:B:279:ILE:HG23	1:B:376:ILE:HG23	1.99	0.45
1:B:295:PRO:HB3	1:B:328:ILE:HD11	1.98	0.45
1:D:312:ALA:HB1	1:D:340:CMH:CM	2.47	0.45
1:C:116:VAL:HB	1:C:151:ILE:HG12	1.99	0.45
1:C:118:ILE:HB	1:C:153:PRO:HA	1.99	0.45
1:B:288:ILE:CB	7:B:1474:5GP:HN22	2.30	0.45
1:B:407:ASP:HB2	1:B:444:LEU:HD22	1.98	0.45
1:D:69:HIS:HE1	1:D:103:HIS:CE1	2.35	0.45
1:C:10:ILE:HD13	1:C:87:LEU:HB2	1.98	0.45
1:D:275:THR:HG22	1:D:347:LYS:HD3	1.98	0.45
1:D:80:ALA:HB1	1:D:112:ILE:HD11	1.99	0.45
1:B:285:ILE:HD13	1:B:291:TYR:HB3	1.99	0.45
1:C:135:ILE:O	1:C:139:ILE:HG13	2.16	0.45
1:D:363:LEU:HA	1:D:364:PRO:HD3	1.77	0.45
6:C:1480:DXC:H243	6:C:1480:DXC:H221	1.72	0.45
1:A:345:GLU:HG2	1:A:346:GLU:HG3	1.99	0.45
1:A:419:LEU:HD12	1:A:445:LEU:HD11	1.98	0.44
1:D:90:VAL:HG21	1:D:136:MET:HE1	1.98	0.44
1:A:136:MET:CE	1:A:139:ILE:HD12	2.47	0.44
1:A:278:LYS:HG3	1:A:381:PRO:HB3	2.00	0.44
1:A:190:LEU:HD22	1:A:203:VAL:HB	2.00	0.44
1:A:118:ILE:HB	1:A:153:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:THR:HA	1:C:324:GLU:HA	1.99	0.44
6:C:1477:DXC:H212	6:C:1477:DXC:H161	1.74	0.44
1:B:131:ARG:O	1:B:135:ILE:HG13	2.17	0.44
1:A:212:VAL:HG23	1:A:242:ALA:HB3	1.99	0.44
1:D:313:VAL:HA	1:D:314:PRO:HD3	1.78	0.44
1:A:83:ILE:HG13	1:A:112:ILE:HD13	1.99	0.44
6:C:1477:DXC:H82	6:C:1477:DXC:H22	1.83	0.44
1:A:296:LYS:HB3	1:A:296:LYS:HE2	1.66	0.44
1:B:89:VAL:HA	1:B:117:VAL:O	2.17	0.44
1:A:131:ARG:O	1:A:135:ILE:HG13	2.18	0.44
1:D:351:GLU:HG2	1:D:354:ASP:CG	2.38	0.44
1:D:109:HIS:CG	1:D:373:HIS:CE1	3.06	0.44
1:D:405:VAL:HG11	1:D:444:LEU:HB3	1.98	0.44
1:B:276:VAL:HG11	1:B:379:PHE:CD1	2.53	0.44
1:B:405:VAL:HG11	1:B:444:LEU:HD13	2.00	0.44
1:A:185:TYR:CE2	1:A:187:LYS:HB2	2.52	0.44
1:C:360:ARG:O	1:C:369:ARG:HB3	2.18	0.44
1:B:6:ILE:HD13	1:B:59:TYR:HD1	1.82	0.44
1:C:406:ILE:HD11	1:C:449:PHE:CZ	2.53	0.44
1:A:286:SER:OG	1:A:372:GLY:HA2	2.17	0.44
1:C:9:GLY:HA2	1:C:64:VAL:HB	2.00	0.44
1:B:397:VAL:O	1:B:456:ARG:N	2.51	0.43
1:C:300:HIS:ND1	1:C:361:LEU:HD12	2.33	0.43
1:A:70:ALA:CB	1:A:365:PRO:HB3	2.48	0.43
1:D:186:PHE:HE1	1:D:207:ILE:HD13	1.82	0.43
1:C:292:ASN:OD1	1:C:294:THR:HG22	2.18	0.43
1:D:43:ARG:HH22	1:D:230:ARG:HD3	1.82	0.43
1:D:426:ILE:HB	1:D:431:ILE:HG12	2.00	0.43
1:A:220:VAL:HG11	1:A:260:ILE:HD11	2.00	0.43
1:A:328:ILE:HG21	1:A:467:TRP:CD1	2.53	0.43
1:C:221:LEU:HD23	1:C:224:ASN:HA	2.01	0.43
1:D:463:ARG:HE	1:D:465:ARG:CZ	2.31	0.43
1:C:380:LYS:HA	1:C:381:PRO:HD3	1.87	0.43
1:C:36:LYS:O	1:C:38:PRO:HD3	2.19	0.43
1:C:79:ALA:O	1:C:83:ILE:HG13	2.19	0.43
1:B:360:ARG:NH1	1:B:371:CMH:SG	2.92	0.43
1:D:442:LYS:HA	1:D:442:LYS:HD3	1.73	0.43
6:C:1479:DXC:H10	6:C:1479:DXC:H61	1.78	0.43
1:C:293:LEU:HD11	1:C:299:VAL:HG11	2.00	0.43
1:D:9:GLY:HA2	1:D:64:VAL:O	2.18	0.43
1:D:34:HIS:NE2	1:D:235:PHE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:VAL:HG13	1:D:266:LEU:HD13	1.99	0.43
1:C:82:ILE:HD11	1:C:208:ASN:HA	1.99	0.43
1:B:24:VAL:O	1:B:28:ILE:HG22	2.19	0.43
1:C:284:LYS:HE3	5:C:1471:SO4:O1	2.19	0.43
1:C:39:GLU:H	1:C:39:GLU:HG2	1.60	0.42
1:C:465:ARG:HG2	5:C:1473:SO4:O1	2.19	0.42
1:B:18:LYS:HB2	4:B:1469:GDP:O2B	2.19	0.42
1:C:67:PRO:HG2	1:C:71:ASP:OD2	2.19	0.42
1:C:84:ASP:CG	1:C:180:ARG:HH22	2.22	0.42
1:B:143:THR:HG21	1:B:146:LEU:HB2	2.02	0.42
1:A:135:ILE:O	1:A:139:ILE:HG13	2.20	0.42
6:C:1475:DXC:H221	6:C:1475:DXC:H243	1.76	0.42
6:C:1475:DXC:H182	6:C:1475:DXC:H71	1.87	0.42
1:A:293:LEU:HD13	1:A:329:LEU:HD23	2.02	0.42
1:A:301:LEU:HD11	1:A:356:VAL:HG13	2.02	0.42
1:C:247:ARG:HG3	1:C:247:ARG:HH11	1.84	0.42
1:D:36:LYS:HA	1:D:236:LYS:HB3	2.02	0.42
1:C:218:LEU:HD12	1:C:266:LEU:HD21	2.01	0.42
6:C:1476:DXC:H201	6:C:1476:DXC:H142	1.87	0.42
1:D:34:HIS:CD2	1:D:236:LYS:HB2	2.55	0.42
1:B:308:VAL:HA	1:B:309:PRO:HD3	1.84	0.42
1:C:165:LEU:O	1:C:169:ILE:HG13	2.20	0.42
1:B:105:LEU:HB3	1:B:370:ILE:HD11	2.02	0.42
1:B:424:ILE:HD12	1:B:459:VAL:HG11	2.01	0.42
6:B:1473:DXC:H13	6:B:1473:DXC:H242	2.02	0.42
1:B:285:ILE:HG13	1:B:371:CMH:O	2.19	0.42
1:B:134:MET:SD	1:D:94:GLU:HG2	2.60	0.42
1:B:60:ARG:HD3	1:B:235:PHE:CE2	2.54	0.42
1:C:207:ILE:HG22	1:C:244:ALA:HA	2.01	0.42
1:C:188:MET:HA	1:C:189:PRO:HD2	1.92	0.42
1:A:322:LYS:HG3	1:A:323:THR:H	1.84	0.42
1:D:74:ARG:O	1:D:307:ILE:HB	2.20	0.41
1:A:285:ILE:HG23	1:A:291:TYR:CD2	2.55	0.41
1:D:6:ILE:HD11	1:D:61:ILE:HG12	2.00	0.41
1:D:293:LEU:HG	1:D:314:PRO:HG3	2.02	0.41
1:A:240:MET:CE	1:B:96:PRO:HD2	2.50	0.41
1:B:376:ILE:HG21	1:B:379:PHE:CE1	2.54	0.41
1:C:360:ARG:NH2	1:C:362:ASP:OD2	2.48	0.41
1:B:140:LEU:O	1:B:143:THR:HB	2.19	0.41
1:B:375:LEU:HA	1:B:375:LEU:HD23	1.86	0.41
1:D:362:ASP:O	1:D:364:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:PHE:CE1	1:A:453:VAL:HG21	2.55	0.41
1:D:170:ILE:HG22	1:D:174:ASN:ND2	2.35	0.41
1:C:108:ASP:CG	1:C:143:THR:HB	2.41	0.41
1:C:147:LYS:HE2	1:C:147:LYS:HB2	1.77	0.41
1:D:148:ASN:OD1	1:D:148:ASN:N	2.43	0.41
1:B:77:VAL:HA	1:B:110:PHE:CE2	2.55	0.41
1:C:169:ILE:O	1:C:173:LEU:HG	2.21	0.41
6:C:1478:DXC:H61	6:C:1478:DXC:H10	1.89	0.41
1:A:85:LEU:HD12	1:A:113:PRO:O	2.21	0.41
1:D:247:ARG:HA	1:D:247:ARG:HD2	1.90	0.41
1:D:32:SER:O	1:D:55:LYS:N	2.46	0.41
1:A:360:ARG:CZ	1:A:363:LEU:HD21	2.51	0.41
6:C:1477:DXC:H201	6:C:1477:DXC:H142	1.63	0.41
1:C:406:ILE:HD11	1:C:449:PHE:HZ	1.86	0.41
1:D:49:ILE:H	1:D:49:ILE:HG12	1.61	0.41
1:C:184:SER:OG	1:C:209:LYS:HB2	2.20	0.41
1:C:-2:ARG:HA	1:C:-1:PRO:HD3	1.91	0.41
1:D:43:ARG:HD2	1:D:231:SER:HB2	2.03	0.41
1:B:361:LEU:HA	1:B:369:ARG:HD2	2.02	0.41
1:B:363:LEU:HA	1:B:363:LEU:HD22	1.94	0.41
1:A:70:ALA:HB1	1:A:369:ARG:NH2	2.36	0.41
1:D:8:LEU:HD12	1:D:85:LEU:O	2.21	0.41
1:D:358:ILE:HD13	1:D:371:CMH:CM	2.51	0.41
1:C:3:PHE:HB2	1:C:60:ARG:CZ	2.51	0.40
1:D:96:PRO:HG3	1:D:136:MET:SD	2.61	0.40
6:C:1475:DXC:H161	6:C:1475:DXC:H211	1.81	0.40
1:A:302:ASN:HB2	1:A:357:LEU:HB3	2.03	0.40
1:B:127:GLU:O	1:B:131:ARG:HG3	2.21	0.40
1:C:89:VAL:HB	1:C:119:THR:HG21	2.03	0.40
1:D:80:ALA:HB1	1:D:112:ILE:CD1	2.51	0.40
1:D:361:LEU:H	1:D:361:LEU:HG	1.57	0.40
1:D:73:ILE:H	1:D:73:ILE:HG13	1.62	0.40
1:A:19:THR:HB	2:A:1469:GNP:O2B	2.20	0.40
1:C:300:HIS:CE1	1:C:361:LEU:HD12	2.57	0.40
1:B:417:GLU:O	1:B:420:ILE:HG12	2.21	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	444/482 (92%)	420 (95%)	24 (5%)	0	100 100
1	B	448/482 (93%)	429 (96%)	19 (4%)	0	100 100
1	C	465/482 (96%)	435 (94%)	28 (6%)	2 (0%)	39 77
1	D	461/482 (96%)	435 (94%)	25 (5%)	1 (0%)	52 86
All	All	1818/1928 (94%)	1719 (95%)	96 (5%)	3 (0%)	52 86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	C	57	GLU
1	C	47	ILE

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	386/412 (94%)	352 (91%)	34 (9%)	12 43
1	B	388/412 (94%)	354 (91%)	34 (9%)	12 43
1	C	402/412 (98%)	358 (89%)	44 (11%)	8 31
1	D	398/412 (97%)	364 (92%)	34 (8%)	13 46
All	All	1574/1648 (96%)	1428 (91%)	146 (9%)	11 39

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	28	ILE
1	A	52	SER
1	A	84	ASP
1	A	90	VAL
1	A	102	GLU
1	A	104	MET
1	A	148	ASN
1	A	150	SER
1	A	152	ILE
1	A	158	THR
1	A	212	VAL
1	A	235	PHE
1	A	250	MET
1	A	252	ILE
1	A	256	ASP
1	A	273	LEU
1	A	313	VAL
1	A	319	THR
1	A	328	ILE
1	A	332	VAL
1	A	348	VAL
1	A	356	VAL
1	A	362	ASP
1	A	366	THR
1	A	377	GLU
1	A	392	LEU
1	A	394	GLU
1	A	424	ILE
1	A	435	ILE
1	A	441	THR
1	A	449	PHE
1	A	458	LYS
1	A	465	ARG
1	B	47	ILE
1	B	62	THR
1	B	90	VAL
1	B	119	THR
1	B	123	ASN
1	B	136	MET
1	B	148	ASN
1	B	163	ASP
1	B	164	GLU

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Mol	Chain	Res	Type
1	B	183	GLU
1	B	208	ASN
1	B	212	VAL
1	B	225	MET
1	B	235	PHE
1	B	241	GLU
1	B	247	ARG
1	B	260	ILE
1	B	262	ARG
1	B	275	THR
1	B	287	ASP
1	B	291	TYR
1	B	300	HIS
1	B	305	MET
1	B	308	VAL
1	B	313	VAL
1	B	319	THR
1	B	344	LEU
1	B	356	VAL
1	B	360	ARG
1	B	363	LEU
1	B	368	LEU
1	B	370	ILE
1	B	394	GLU
1	B	453	VAL
1	C	-2	ARG
1	C	6	ILE
1	C	14	ILE
1	C	52	SER
1	C	71	ASP
1	C	78	SER
1	C	114	ILE
1	C	123	ASN
1	C	126	THR
1	C	142	SER
1	C	148	ASN
1	C	150	SER
1	C	158	THR
1	C	171	THR
1	C	191	ASP
1	C	218	LEU
1	C	223	ILE

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Mol	Chain	Res	Type
1	C	226	SER
1	C	241	GLU
1	C	255	VAL
1	C	278	LYS
1	C	292	ASN
1	C	293	LEU
1	C	294	THR
1	C	306	LEU
1	C	319	THR
1	C	328	ILE
1	C	332	VAL
1	C	334	SER
1	C	349	LEU
1	C	355	ARG
1	C	357	LEU
1	C	359	THR
1	C	362	ASP
1	C	366	THR
1	C	368	LEU
1	C	369	ARG
1	C	373	HIS
1	C	378	GLU
1	C	391	VAL
1	C	435	ILE
1	C	445	LEU
1	C	446	THR
1	C	456	ARG
1	D	15	ASP
1	D	16	HIS
1	D	36	LYS
1	D	41	GLN
1	D	43	ARG
1	D	45	ILE
1	D	46	THR
1	D	49	ILE
1	D	73	ILE
1	D	74	ARG
1	D	78	SER
1	D	89	VAL
1	D	90	VAL
1	D	128	GLU
1	D	139	ILE

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Mol	Chain	Res	Type
1	D	143	THR
1	D	160	PHE
1	D	162	VAL
1	D	190	LEU
1	D	220	VAL
1	D	226	SER
1	D	233	GLN
1	D	235	PHE
1	D	277	ASP
1	D	289	PHE
1	D	333	ILE
1	D	334	SER
1	D	348	VAL
1	D	361	LEU
1	D	362	ASP
1	D	363	LEU
1	D	368	LEU
1	D	435	ILE
1	D	453	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	300	HIS
1	C	233	GLN
1	D	69	HIS
1	D	233	GLN
1	D	373	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CMH	A	264	1	5,7,8	0.55	0	2,7,9	1.32	0
1	CMH	A	338	1	5,7,8	0.52	0	2,7,9	1.51	0
1	CMH	A	340	1	5,7,8	0.58	0	2,7,9	1.62	0
1	CMH	A	371	1	5,7,8	0.51	0	2,7,9	1.60	1 (50%)
1	CMH	B	264	1	5,7,8	0.70	0	2,7,9	1.67	0
1	CMH	B	338	1	5,7,8	0.53	0	2,7,9	1.21	0
1	CMH	B	340	1	5,7,8	0.49	0	2,7,9	1.49	0
1	CMH	B	371	1	5,7,8	0.48	0	2,7,9	1.82	1 (50%)
1	CMH	C	264	1	5,7,8	0.60	0	2,7,9	1.46	0
1	CMH	C	338	1	5,7,8	0.56	0	2,7,9	1.25	0
1	CMH	C	340	1	5,7,8	0.76	0	2,7,9	1.42	0
1	CMH	C	371	1	5,7,8	0.63	0	2,7,9	1.33	0
1	CMH	D	264	1	5,7,8	0.56	0	2,7,9	1.28	0
1	CMH	D	338	1	5,7,8	0.56	0	2,7,9	1.64	1 (50%)
1	CMH	D	340	1	5,7,8	0.60	0	2,7,9	1.28	0
1	CMH	D	371	1	5,7,8	0.56	0	2,7,9	1.48	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
1	CMH	A	264	1	-	0/0/6/8	0/0/0/0
1	CMH	A	338	1	-	0/0/6/8	0/0/0/0
1	CMH	A	340	1	-	0/0/6/8	0/0/0/0
1	CMH	A	371	1	-	0/0/6/8	0/0/0/0
1	CMH	B	264	1	-	0/0/6/8	0/0/0/0
1	CMH	B	338	1	-	0/0/6/8	0/0/0/0
1	CMH	B	340	1	-	0/0/6/8	0/0/0/0
1	CMH	B	371	1	-	0/0/6/8	0/0/0/0
1	CMH	C	264	1	-	0/0/6/8	0/0/0/0
1	CMH	C	338	1	-	0/0/6/8	0/0/0/0
1	CMH	C	340	1	-	0/0/6/8	0/0/0/0
1	CMH	C	371	1	-	0/0/6/8	0/0/0/0
1	CMH	D	264	1	-	0/0/6/8	0/0/0/0
1	CMH	D	338	1	-	0/0/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CMH	D	340	1	-	0/0/6/8	0/0/0/0
1	CMH	D	371	1	-	0/0/6/8	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	338	CMH	O-C-CA	-2.31	119.46	125.49
1	A	371	CMH	O-C-CA	-2.13	119.94	125.49
1	B	371	CMH	O-C-CA	-2.02	120.24	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	338	CMH	1	0
1	A	340	CMH	2	0
1	B	371	CMH	2	0
1	C	338	CMH	1	0
1	C	340	CMH	2	0
1	C	371	CMH	3	0
1	D	338	CMH	2	0
1	D	340	CMH	4	0
1	D	371	CMH	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	GNP	A	1469	3	28,34,34	1.86	5 (17%)	33,54,54	2.40	8 (24%)
4	GDP	B	1469	3	23,30,30	1.20	2 (8%)	30,47,47	1.78	6 (20%)
5	SO4	B	1471	-	4,4,4	0.11	0	6,6,6	0.10	0
5	SO4	B	1472	-	4,4,4	0.19	0	6,6,6	0.16	0
6	DXC	B	1473	-	28,31,31	1.31	3 (10%)	46,49,49	2.07	12 (26%)
7	5GP	B	1474	-	21,26,26	0.53	0	25,40,40	1.71	6 (24%)
5	SO4	C	1471	-	4,4,4	0.46	0	6,6,6	0.44	0
5	SO4	C	1472	-	4,4,4	0.16	0	6,6,6	0.15	0
5	SO4	C	1473	-	4,4,4	0.13	0	6,6,6	0.15	0
6	DXC	C	1475	-	28,31,31	1.59	4 (14%)	46,49,49	2.21	15 (32%)
6	DXC	C	1476	-	28,31,31	1.47	5 (17%)	46,49,49	1.86	12 (26%)
6	DXC	C	1477	-	28,31,31	1.58	6 (21%)	46,49,49	1.88	12 (26%)
6	DXC	C	1478	-	28,31,31	1.33	5 (17%)	46,49,49	1.89	14 (30%)
6	DXC	C	1479	-	28,31,31	1.52	7 (25%)	46,49,49	2.13	18 (39%)
6	DXC	C	1480	-	28,31,31	1.58	7 (25%)	46,49,49	2.08	16 (34%)
5	SO4	C	1481	-	4,4,4	0.08	0	6,6,6	0.09	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	GNP	A	1469	3	-	0/12/38/38	0/3/3/3
4	GDP	B	1469	3	-	0/12/32/32	0/3/3/3
5	SO4	B	1471	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1472	-	-	0/0/0/0	0/0/0/0
6	DXC	B	1473	-	-	0/7/71/71	0/4/4/4
7	5GP	B	1474	-	-	0/6/26/26	0/3/3/3
5	SO4	C	1471	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1472	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1473	-	-	0/0/0/0	0/0/0/0
6	DXC	C	1475	-	-	0/7/71/71	0/4/4/4
6	DXC	C	1476	-	-	0/7/71/71	0/4/4/4
6	DXC	C	1477	-	-	0/7/71/71	0/4/4/4
6	DXC	C	1478	-	-	0/7/71/71	0/4/4/4
6	DXC	C	1479	-	-	0/7/71/71	0/4/4/4
6	DXC	C	1480	-	-	0/7/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	C	1481	-	-	0/0/0/0	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1469	GNP	PB-O3A	-4.81	1.53	1.59
6	C	1475	DXC	C12-C13	-4.55	1.47	1.54
6	C	1477	DXC	C12-C13	-3.80	1.48	1.54
6	C	1477	DXC	C18-C4	-3.65	1.47	1.54
6	C	1480	DXC	C18-C4	-3.58	1.47	1.54
6	C	1476	DXC	C12-C13	-3.35	1.49	1.54
6	C	1479	DXC	C18-C4	-3.13	1.48	1.54
6	C	1476	DXC	O1-C13	-3.07	1.38	1.43
6	C	1480	DXC	C12-C13	-3.02	1.49	1.54
6	B	1473	DXC	C12-C13	-2.98	1.49	1.54
6	C	1478	DXC	C18-C4	-2.94	1.48	1.54
6	C	1479	DXC	C12-C13	-2.89	1.50	1.54
6	C	1477	DXC	C4-C10	-2.83	1.50	1.56
6	C	1475	DXC	O1-C13	-2.83	1.38	1.43
6	C	1476	DXC	C12-C11	-2.80	1.50	1.55
6	C	1476	DXC	C20-C12	-2.80	1.49	1.54
6	C	1475	DXC	C20-C12	-2.79	1.49	1.54
2	A	1469	GNP	PB-O2B	-2.78	1.49	1.56
6	B	1473	DXC	C18-C4	-2.77	1.49	1.54
6	C	1475	DXC	C12-C11	-2.77	1.50	1.55
6	C	1477	DXC	C20-C12	-2.67	1.50	1.54
6	C	1480	DXC	C12-C11	-2.64	1.50	1.55
6	C	1480	DXC	C5-C4	-2.57	1.49	1.54
6	C	1478	DXC	C12-C11	-2.51	1.51	1.55
6	B	1473	DXC	C4-C10	-2.44	1.51	1.56
6	C	1479	DXC	O1-C13	-2.37	1.39	1.43
6	C	1478	DXC	C12-C13	-2.34	1.50	1.54
6	C	1479	DXC	C4-C3	-2.34	1.51	1.55
6	C	1478	DXC	O1-C13	-2.34	1.39	1.43
6	C	1476	DXC	C18-C4	-2.27	1.50	1.54
6	C	1480	DXC	C4-C10	-2.24	1.51	1.56
6	C	1479	DXC	C20-C12	-2.22	1.50	1.54
6	C	1480	DXC	C4-C3	-2.22	1.51	1.55
6	C	1477	DXC	O1-C13	-2.20	1.39	1.43
6	C	1479	DXC	C12-C11	-2.19	1.51	1.55
6	C	1478	DXC	C20-C12	-2.12	1.50	1.54
6	C	1480	DXC	O1-C13	-2.12	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1479	DXC	C4-C10	-2.06	1.52	1.56
6	C	1477	DXC	C12-C11	-2.02	1.52	1.55
2	A	1469	GNP	C8-N7	-2.02	1.30	1.34
4	B	1469	GDP	C5-C4	3.02	1.47	1.40
2	A	1469	GNP	C6-N1	3.62	1.39	1.33
4	B	1469	GDP	C6-C5	3.81	1.48	1.41
2	A	1469	GNP	PG-O1G	4.90	1.51	1.46

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1469	GNP	C5-C6-N1	-8.75	111.63	123.59
6	C	1478	DXC	C10-C14-C13	-5.92	106.89	114.36
6	C	1475	DXC	C15-C11-C12	-5.34	98.29	103.60
6	C	1475	DXC	C3-C2-C1	-4.95	105.55	112.91
6	B	1473	DXC	C22-C21-C19	-4.90	108.97	114.75
6	C	1477	DXC	C10-C14-C13	-4.90	108.17	114.36
6	C	1476	DXC	C22-C21-C19	-4.90	108.98	114.75
6	C	1479	DXC	C18-C4-C3	-4.87	101.64	110.25
6	C	1479	DXC	C6-C5-C4	-4.78	104.30	112.84
6	C	1479	DXC	C24-C19-C17	-4.48	105.49	112.96
6	C	1475	DXC	C17-C12-C13	-4.46	113.73	117.68
6	C	1477	DXC	C14-C13-C12	-4.41	106.72	111.20
6	C	1476	DXC	C18-C4-C3	-4.40	102.49	110.25
6	C	1480	DXC	C18-C4-C5	-4.37	100.84	108.20
6	B	1473	DXC	C6-C5-C4	-4.36	105.05	112.84
6	B	1473	DXC	C11-C9-C10	-4.27	103.45	109.06
6	C	1475	DXC	O1-C13-C12	-4.19	104.31	111.11
4	B	1469	GDP	C5-C6-N1	-4.16	117.90	123.59
7	B	1474	5GP	N3-C2-N1	-4.00	121.35	127.44
6	C	1478	DXC	C7-C8-C9	-3.99	104.96	112.10
6	C	1477	DXC	C11-C9-C10	-3.90	103.93	109.06
6	B	1473	DXC	C14-C10-C4	-3.78	109.86	113.79
6	B	1473	DXC	C5-C6-C1	-3.76	104.34	110.43
6	C	1477	DXC	C7-C8-C9	-3.70	105.49	112.10
6	C	1478	DXC	C22-C21-C19	-3.52	110.60	114.75
6	C	1476	DXC	C10-C14-C13	-3.47	109.98	114.36
6	C	1480	DXC	C17-C12-C13	-3.43	114.64	117.68
6	C	1475	DXC	C18-C4-C3	-3.42	104.20	110.25
6	C	1480	DXC	C11-C12-C13	-3.40	104.34	107.39
2	A	1469	GNP	O3G-PG-O1G	-3.39	104.47	113.49
6	C	1476	DXC	C4-C10-C9	-3.38	108.63	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1480	DXC	C10-C14-C13	-3.38	110.10	114.36
6	C	1475	DXC	C11-C9-C10	-3.33	104.67	109.06
4	B	1469	GDP	C4-C5-N7	-3.33	106.42	109.48
6	C	1479	DXC	C7-C8-C9	-3.32	106.16	112.10
6	C	1477	DXC	C11-C12-C13	-3.32	104.42	107.39
4	B	1469	GDP	N3-C2-N1	-3.28	122.45	127.44
6	C	1480	DXC	C16-C15-C11	-3.24	98.61	105.12
6	C	1479	DXC	C15-C11-C9	-3.21	113.95	119.03
6	C	1475	DXC	C5-C6-C1	-3.21	105.23	110.43
6	B	1473	DXC	C5-C4-C10	-3.18	106.32	111.45
6	C	1480	DXC	C24-C19-C21	-3.13	105.13	110.35
6	C	1476	DXC	C7-C8-C9	-3.13	106.51	112.10
6	C	1478	DXC	C3-C2-C1	-3.11	108.29	112.91
6	C	1480	DXC	C7-C8-C9	-3.10	106.56	112.10
4	B	1469	GDP	C6-C5-C4	-3.09	117.20	120.90
6	C	1479	DXC	C11-C9-C10	-3.09	104.99	109.06
6	C	1478	DXC	C12-C17-C19	-3.07	115.76	119.50
6	C	1479	DXC	C14-C10-C4	-3.05	110.62	113.79
6	B	1473	DXC	C18-C4-C3	-3.05	104.87	110.25
6	C	1475	DXC	C6-C5-C4	-3.02	107.45	112.84
2	A	1469	GNP	PA-O3A-PB	-2.88	122.99	132.67
7	B	1474	5GP	O5'-P-O1P	-2.80	100.01	107.14
6	C	1479	DXC	C10-C14-C13	-2.79	110.83	114.36
7	B	1474	5GP	C5-C6-N1	-2.78	119.79	123.59
6	C	1478	DXC	C16-C15-C11	-2.74	99.60	105.12
6	C	1480	DXC	O1-C13-C12	-2.72	106.70	111.11
6	C	1477	DXC	C2-C3-C7	-2.68	106.66	111.66
6	C	1479	DXC	C12-C17-C19	-2.65	116.27	119.50
6	C	1480	DXC	C4-C10-C9	-2.63	109.47	112.40
6	C	1476	DXC	C15-C11-C12	-2.62	101.00	103.60
6	B	1473	DXC	C24-C19-C21	-2.61	105.99	110.35
6	C	1480	DXC	C3-C2-C1	-2.61	109.03	112.91
6	C	1479	DXC	C14-C13-C12	-2.60	108.56	111.20
6	C	1479	DXC	C15-C11-C12	-2.53	101.08	103.60
6	C	1479	DXC	C4-C10-C9	-2.52	109.59	112.40
6	C	1478	DXC	C6-C5-C4	-2.48	108.42	112.84
6	C	1478	DXC	C24-C19-C21	-2.47	106.24	110.35
6	C	1475	DXC	C2-C1-C6	-2.46	107.39	110.52
6	C	1475	DXC	C16-C15-C11	-2.44	100.21	105.12
4	B	1469	GDP	PA-O3A-PB	-2.36	124.76	132.67
6	C	1476	DXC	C3-C2-C1	-2.34	109.43	112.91
6	C	1475	DXC	C18-C4-C5	-2.33	104.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1480	DXC	C22-C21-C19	-2.31	112.03	114.75
6	C	1477	DXC	C16-C15-C11	-2.28	100.54	105.12
6	C	1475	DXC	C2-C3-C4	-2.25	110.17	112.66
2	A	1469	GNP	N3-C2-N1	-2.25	124.02	127.44
6	C	1476	DXC	C15-C11-C9	-2.21	115.54	119.03
7	B	1474	5GP	C4-C5-N7	-2.18	107.47	109.48
6	C	1477	DXC	C20-C12-C13	-2.17	106.98	109.09
6	C	1478	DXC	C2-C3-C7	-2.16	107.63	111.66
6	C	1478	DXC	C8-C7-C3	-2.12	107.62	111.92
6	C	1478	DXC	C2-C1-C6	-2.10	107.85	110.52
6	C	1475	DXC	C12-C17-C19	-2.09	116.96	119.50
6	C	1479	DXC	C20-C12-C13	-2.01	107.13	109.09
7	B	1474	5GP	O3P-P-O2P	2.02	115.07	107.38
6	B	1473	DXC	C2-C3-C4	2.02	114.88	112.66
6	C	1477	DXC	C12-C11-C9	2.03	117.08	114.74
2	A	1469	GNP	O3A-PA-O5'	2.09	108.48	102.94
6	C	1476	DXC	C5-C6-C1	2.17	113.95	110.43
6	C	1478	DXC	C21-C19-C17	2.19	114.85	110.24
6	C	1480	DXC	C8-C9-C10	2.22	113.11	110.46
6	B	1473	DXC	C15-C11-C12	2.22	105.81	103.60
6	C	1480	DXC	C10-C4-C3	2.24	111.99	108.67
6	C	1480	DXC	O2-C1-C2	2.24	114.33	109.86
6	C	1479	DXC	C11-C12-C13	2.35	109.49	107.39
6	C	1478	DXC	C10-C4-C3	2.35	112.16	108.67
6	C	1479	DXC	C18-C4-C10	2.36	114.71	111.18
6	C	1477	DXC	C10-C4-C3	2.62	112.55	108.67
6	C	1478	DXC	C8-C9-C10	2.63	113.61	110.46
6	C	1477	DXC	C20-C12-C11	2.68	115.44	111.22
2	A	1469	GNP	O3G-PG-O2G	2.77	115.78	107.58
6	C	1476	DXC	C17-C12-C13	2.80	120.16	117.68
6	C	1479	DXC	C5-C4-C3	2.81	112.43	107.81
6	B	1473	DXC	C20-C12-C11	2.85	115.72	111.22
6	C	1479	DXC	C8-C9-C10	3.02	114.08	110.46
6	C	1480	DXC	C5-C4-C10	3.03	116.34	111.45
6	C	1477	DXC	C17-C12-C11	3.05	103.14	100.05
6	C	1479	DXC	C10-C4-C3	3.08	113.24	108.67
6	C	1475	DXC	C17-C12-C11	3.12	103.21	100.05
6	C	1476	DXC	C8-C9-C10	3.31	114.42	110.46
6	C	1476	DXC	C10-C4-C3	3.37	113.66	108.67
7	B	1474	5GP	C6-N1-C2	3.51	120.81	115.94
2	A	1469	GNP	O2B-PB-O1B	3.51	117.33	110.00
6	C	1475	DXC	C18-C4-C10	3.57	116.53	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1473	DXC	C10-C4-C3	4.23	114.94	108.67
4	B	1469	GDP	C6-N1-C2	4.72	122.49	115.94
6	C	1480	DXC	C20-C12-C13	4.96	113.93	109.09
2	A	1469	GNP	C6-N1-C2	6.42	124.85	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1469	GNP	2	0
4	B	1469	GDP	2	0
5	B	1471	SO4	1	0
5	B	1472	SO4	1	0
6	B	1473	DXC	4	0
7	B	1474	5GP	2	0
5	C	1471	SO4	1	0
5	C	1473	SO4	1	0
6	C	1475	DXC	5	0
6	C	1476	DXC	2	0
6	C	1477	DXC	3	0
6	C	1478	DXC	2	0
6	C	1479	DXC	1	0
6	C	1480	DXC	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	448/482 (92%)	1.10	103 (22%) 1 1	107, 205, 299, 372	0
1	B	452/482 (93%)	0.79	72 (15%) 3 2	80, 152, 347, 414	0
1	C	467/482 (96%)	0.27	21 (4%) 37 36	74, 123, 227, 308	0
1	D	463/482 (96%)	2.21	202 (43%) 0 1	140, 274, 369, 416	0
All	All	1830/1928 (94%)	1.09	398 (21%) 1 1	74, 188, 338, 416	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	453	VAL	13.0
1	D	401	LYS	12.2
1	D	78	SER	11.2
1	B	404	THR	11.2
1	D	438	THR	11.1
1	D	442	LYS	11.0
1	D	250	MET	10.9
1	B	432	VAL	10.7
1	A	81	ASP	10.6
1	D	441	THR	10.4
1	D	412	SER	10.4
1	B	418	LYS	9.3
1	D	333	ILE	9.2
1	D	399	ILE	9.0
1	D	65	ASP	8.9
1	D	304	GLY	8.8
1	D	467	TRP	8.7
1	D	79	ALA	8.5
1	B	441	THR	8.3
1	D	242	ALA	8.2
1	D	390	GLU	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	406	ILE	8.1
1	A	449	PHE	7.9
1	A	405	VAL	7.7
1	D	402	GLY	7.7
1	B	461	LEU	7.7
1	D	382	ILE	7.6
1	D	392	LEU	7.6
1	D	320	PHE	7.5
1	D	330	ASN	7.4
1	D	400	ASP	7.3
1	B	450	SER	7.3
1	D	69	HIS	7.3
1	B	330	ASN	7.3
1	D	414	VAL	7.2
1	D	251	ALA	7.2
1	D	416	ALA	7.1
1	B	405	VAL	7.0
1	D	391	VAL	6.9
1	A	406	ILE	6.9
1	D	31	THR	6.8
1	D	256	ASP	6.6
1	D	179	ILE	6.6
1	A	404	THR	6.6
1	D	415	ALA	6.6
1	D	311	VAL	6.6
1	D	16	HIS	6.5
1	D	426	ILE	6.5
1	D	431	ILE	6.4
1	A	434	LYS	6.4
1	D	425	SER	6.4
1	D	38	PRO	6.4
1	D	405	VAL	6.3
1	D	66	ALA	6.3
1	B	396	LYS	6.2
1	D	322	LYS	6.2
1	B	433	GLY	6.2
1	A	441	THR	6.2
1	B	460	ILE	6.1
1	A	257	ALA	6.1
1	D	173	LEU	6.0
1	B	428	GLY	6.0
1	D	417	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	411	GLN	6.0
1	D	332	VAL	5.9
1	D	17	GLY	5.8
1	B	449	PHE	5.8
1	D	172	THR	5.7
1	D	295	PRO	5.6
1	D	429	LYS	5.6
1	A	225	MET	5.6
1	D	329	LEU	5.5
1	C	35	ASP	5.5
1	D	318	VAL	5.5
1	A	448	GLU	5.4
1	D	40	SER	5.3
1	D	452	ASN	5.3
1	A	304	GLY	5.3
1	A	433	GLY	5.3
1	A	259	GLN	5.3
1	B	427	GLU	5.2
1	D	428	GLY	5.2
1	D	439	PHE	5.2
1	D	413	LYS	5.2
1	D	45	ILE	5.1
1	B	397	VAL	5.1
1	D	403	ARG	5.1
1	A	397	VAL	5.0
1	D	312	ALA	5.0
1	B	392	LEU	5.0
1	D	464	LEU	4.9
1	A	47	ILE	4.9
1	B	439	PHE	4.9
1	A	198	GLY	4.9
1	A	435	ILE	4.9
1	D	462	ASN	4.9
1	A	46	THR	4.8
1	A	196	ILE	4.8
1	A	424	ILE	4.7
1	A	256	ASP	4.7
1	D	292	ASN	4.7
1	A	422	GLU	4.7
1	D	343	GLU	4.7
1	D	15	ASP	4.7
1	D	430	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	233	GLN	4.6
1	D	316	LYS	4.6
1	D	334	SER	4.6
1	B	440	GLY	4.6
1	A	429	LYS	4.5
1	D	444	LEU	4.5
1	A	439	PHE	4.5
1	D	331	GLU	4.5
1	A	220	VAL	4.5
1	D	440	GLY	4.5
1	A	426	ILE	4.4
1	D	200	GLY	4.4
1	A	452	ASN	4.4
1	D	241	GLU	4.4
1	D	48	ASP	4.4
1	B	445	LEU	4.3
1	C	34	HIS	4.3
1	B	415	ALA	4.3
1	D	321	GLY	4.3
1	D	81	ASP	4.3
1	D	289	PHE	4.3
1	B	424	ILE	4.3
1	A	465	ARG	4.3
1	D	456	ARG	4.3
1	D	212	VAL	4.3
1	A	287	ASP	4.3
1	D	39	GLU	4.3
1	D	178	ILE	4.2
1	D	455	ASN	4.2
1	A	69	HIS	4.2
1	A	389	LYS	4.2
1	B	429	LYS	4.2
1	D	195	PRO	4.2
1	C	32	SER	4.2
1	D	47	ILE	4.2
1	D	259	GLN	4.2
1	B	409	LEU	4.2
1	D	255	VAL	4.2
1	D	424	ILE	4.1
1	A	445	LEU	4.1
1	D	384	ASP	4.1
1	B	414	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	258	LYS	4.1
1	D	249	GLY	4.1
1	B	417	GLU	4.0
1	D	258	LYS	4.0
1	D	328	ILE	4.0
1	A	398	LYS	4.0
1	D	323	THR	4.0
1	D	445	LEU	4.0
1	A	284	LYS	3.9
1	D	169	ILE	3.9
1	A	450	SER	3.9
1	D	388	LYS	3.9
1	D	465	ARG	3.9
1	D	223	ILE	3.9
1	A	380	LYS	3.9
1	D	154	ILE	3.9
1	D	305	MET	3.9
1	D	67	PRO	3.8
1	A	218	LEU	3.8
1	C	430	ASP	3.8
1	D	327	ILE	3.8
1	B	321	GLY	3.8
1	A	197	LYS	3.8
1	D	21	LEU	3.7
1	A	432	VAL	3.7
1	D	325	GLU	3.7
1	D	36	LYS	3.7
1	D	219	LYS	3.7
1	D	389	LYS	3.6
1	B	438	THR	3.6
1	C	323	THR	3.6
1	D	22	SER	3.6
1	B	413	LYS	3.6
1	C	36	LYS	3.6
1	D	436	LYS	3.6
1	A	329	LEU	3.6
1	D	68	GLY	3.6
1	B	455	ASN	3.6
1	D	220	VAL	3.5
1	D	225	MET	3.5
1	B	318	VAL	3.5
1	D	221	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	3.5
1	A	323	THR	3.5
1	B	399	ILE	3.5
1	D	19	THR	3.4
1	D	122	ASP	3.4
1	A	413	LYS	3.4
1	D	30	SER	3.4
1	A	451	GLY	3.4
1	D	380	LYS	3.4
1	D	407	ASP	3.4
1	B	323	THR	3.4
1	A	428	GLY	3.4
1	D	269	LYS	3.4
1	D	409	LEU	3.3
1	D	397	VAL	3.3
1	A	324	GLU	3.3
1	D	218	LEU	3.3
1	D	461	LEU	3.3
1	D	13	HIS	3.3
1	B	362	ASP	3.3
1	D	345	GLU	3.3
1	A	396	LYS	3.3
1	D	155	SER	3.3
1	A	336	ASN	3.3
1	B	322	LYS	3.3
1	A	407	ASP	3.3
1	B	398	LYS	3.2
1	D	290	LYS	3.2
1	B	426	ILE	3.2
1	D	4	LYS	3.2
1	A	447	ALA	3.2
1	B	447	ALA	3.2
1	C	402	GLY	3.2
1	D	170	ILE	3.2
1	A	446	THR	3.2
1	A	436	LYS	3.2
1	D	454	GLU	3.2
1	B	403	ARG	3.2
1	A	242	ALA	3.2
1	D	393	ARG	3.2
1	D	232	ILE	3.1
1	A	260	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	286	SER	3.1
1	A	423	GLU	3.1
1	A	282	LYS	3.1
1	B	1	MET	3.1
1	D	20	THR	3.1
1	D	326	ASN	3.1
1	D	314	PRO	3.1
1	D	437	GLY	3.1
1	A	388	LYS	3.0
1	B	434	LYS	3.0
1	A	326	ASN	3.0
1	D	313	VAL	3.0
1	A	319	THR	3.0
1	A	321	GLY	3.0
1	D	120	LYS	3.0
1	B	394	GLU	3.0
1	D	59	TYR	3.0
1	A	419	LEU	3.0
1	D	28	ILE	3.0
1	A	78	SER	2.9
1	D	443	GLY	2.9
1	A	200	GLY	2.9
1	B	435	ILE	2.9
1	D	335	GLY	2.9
1	B	453	VAL	2.9
1	D	419	LEU	2.9
1	D	243	LYS	2.9
1	A	438	THR	2.9
1	B	393	ARG	2.9
1	D	191	ASP	2.9
1	D	211	ILE	2.8
1	D	119	THR	2.8
1	D	468	GLY	2.8
1	A	255	VAL	2.8
1	B	406	ILE	2.8
1	A	195	PRO	2.8
1	C	37	LEU	2.8
1	B	467	TRP	2.8
1	D	294	THR	2.8
1	B	402	GLY	2.8
1	D	217	GLU	2.8
1	B	308	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	458	LYS	2.8
1	A	459	VAL	2.8
1	B	416	ALA	2.8
1	D	385	LEU	2.7
1	B	459	VAL	2.7
1	B	320	PHE	2.7
1	D	230	ARG	2.7
1	C	414	VAL	2.7
1	C	322	LYS	2.7
1	A	320	PHE	2.7
1	D	377	GLU	2.7
1	A	281	ALA	2.7
1	D	156	ALA	2.7
1	B	458	LYS	2.7
1	D	180	ARG	2.7
1	D	459	VAL	2.7
1	A	431	ILE	2.6
1	D	254	GLY	2.6
1	A	317	LYS	2.6
1	A	201	THR	2.6
1	D	383	LYS	2.6
1	A	444	LEU	2.6
1	A	211	ILE	2.6
1	B	311	VAL	2.6
1	A	289	PHE	2.6
1	D	50	GLY	2.6
1	B	324	GLU	2.6
1	D	3	PHE	2.6
1	D	43	ARG	2.6
1	B	109	HIS	2.6
1	D	378	GLU	2.6
1	B	464	LEU	2.5
1	A	430	ASP	2.5
1	A	409	LEU	2.5
1	B	457	ASP	2.5
1	B	454	GLU	2.5
1	C	409	LEU	2.5
1	C	442	LYS	2.5
1	D	418	LYS	2.5
1	B	456	ARG	2.5
1	D	177	GLU	2.5
1	A	271	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	410	ALA	2.5
1	C	13	HIS	2.5
1	D	228	LYS	2.5
1	D	350	ALA	2.5
1	C	435	ILE	2.5
1	B	389	LYS	2.5
1	D	347	LYS	2.5
1	A	212	VAL	2.5
1	B	29	ALA	2.5
1	A	440	GLY	2.5
1	A	442	LYS	2.5
1	A	379	PHE	2.5
1	D	356	VAL	2.5
1	D	76	VAL	2.5
1	D	80	ALA	2.4
1	D	379	PHE	2.4
1	A	199	ALA	2.4
1	D	52	SER	2.4
1	A	390	GLU	2.4
1	D	25	LEU	2.4
1	A	418	LYS	2.4
1	B	334	SER	2.4
1	D	267	THR	2.4
1	A	385	LEU	2.4
1	D	268	SER	2.4
1	C	269	LYS	2.4
1	D	270	ASP	2.3
1	D	77	VAL	2.3
1	B	298	LYS	2.3
1	D	288	ILE	2.3
1	B	442	LYS	2.3
1	B	462	ASN	2.3
1	C	411	GLN	2.3
1	C	-2	ARG	2.3
1	D	435	ILE	2.3
1	C	467	TRP	2.3
1	D	458	LYS	2.3
1	A	387	ILE	2.3
1	D	196	ILE	2.3
1	D	32	SER	2.3
1	D	257	ALA	2.3
1	D	280	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	460	ILE	2.3
1	D	286	SER	2.3
1	B	400	ASP	2.3
1	B	329	LEU	2.2
1	C	320	PHE	2.2
1	D	248	VAL	2.2
1	D	252	ILE	2.2
1	D	203	VAL	2.2
1	B	423	GLU	2.2
1	D	192	HIS	2.2
1	D	165	LEU	2.2
1	D	319	THR	2.2
1	A	84	ASP	2.2
1	B	419	LEU	2.2
1	B	319	THR	2.2
1	D	262	ARG	2.2
1	D	227	THR	2.2
1	A	453	VAL	2.2
1	A	376	ILE	2.2
1	A	322	LYS	2.1
1	A	464	LEU	2.1
1	A	217	GLU	2.1
1	D	297	MET	2.1
1	A	325	GLU	2.1
1	D	166	LYS	2.1
1	C	319	THR	2.1
1	D	18	LYS	2.1
1	A	378	GLU	2.1
1	A	316	LYS	2.1
1	D	197	LYS	2.1
1	D	296	LYS	2.1
1	A	291	TYR	2.1
1	D	202	VAL	2.1
1	D	381	PRO	2.1
1	A	467	TRP	2.0
1	C	406	ILE	2.0
1	D	342	PHE	2.0
1	A	337	GLU	2.0
1	A	415	ALA	2.0
1	B	388	LYS	2.0
1	D	224	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
1	CMH	D	264	8/9	0.92	0.26	-	241,255,280,281	2
1	CMH	C	264	8/9	0.99	0.16	-	70,108,137,210	0
1	CMH	B	338	8/9	0.92	0.28	-	151,200,232,276	2
1	CMH	A	371	8/9	0.88	0.36	-	168,213,225,228	2
1	CMH	C	371	8/9	0.99	0.25	-	78,109,123,156	2
1	CMH	C	340	8/9	0.98	0.24	-	69,99,124,131	2
1	CMH	B	340	8/9	0.98	0.25	-	160,194,264,332	0
1	CMH	A	264	8/9	0.97	0.17	-	171,215,224,235	2
1	CMH	D	340	8/9	0.90	0.21	-	207,306,312,317	2
1	CMH	A	340	8/9	0.98	0.19	-	169,213,226,240	2
1	CMH	B	264	8/9	1.00	0.17	-	73,89,99,112	2
1	CMH	D	371	8/9	0.98	0.19	-	145,181,227,234	2
1	CMH	D	338	8/9	0.81	0.11	-	180,242,266,268	2
1	CMH	C	338	8/9	0.96	0.18	-	74,109,174,331	2
1	CMH	B	371	8/9	0.93	0.30	-	174,197,251,332	2
1	CMH	A	338	8/9	0.95	0.14	-	174,190,268,307	2

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, 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
5	SO4	B	1472	5/5	0.82	0.89	9.92	139,226,336,344	0
7	5GP	B	1474	24/24	0.81	0.38	1.54	242,294,308,311	0
6	DXC	C	1479	28/28	0.93	0.29	1.19	82,104,174,196	28

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	DXC	C	1477	28/28	0.94	0.31	0.99	91,111,162,182	0
6	DXC	C	1476	28/28	0.92	0.33	0.64	159,168,217,253	0
6	DXC	C	1478	28/28	0.96	0.24	0.57	93,118,158,196	0
5	SO4	C	1471	5/5	0.97	0.22	0.45	101,149,159,220	0
6	DXC	C	1475	28/28	0.96	0.27	0.29	61,95,139,146	0
6	DXC	B	1473	28/28	0.95	0.28	0.28	68,97,134,143	0
4	GDP	B	1469	28/28	0.92	0.21	-0.10	126,197,212,235	0
6	DXC	C	1480	28/28	0.97	0.23	-0.46	63,85,106,127	0
2	GNP	A	1469	32/32	0.97	0.12	-1.00	120,165,202,249	0
5	SO4	B	1471	5/5	0.78	0.18	-	205,213,271,283	0
3	MG	B	1470	1/1	0.98	0.20	-	342,342,342,342	0
5	SO4	C	1473	5/5	0.83	0.14	-	164,166,220,230	5
5	SO4	C	1472	5/5	0.93	0.19	-	133,154,189,210	0
3	MG	A	1470	1/1	0.98	0.07	-	244,244,244,244	0
5	SO4	C	1481	5/5	0.90	1.65	-	172,210,221,235	5

6.5 Other polymers (i)

There are no such residues in this entry.