Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:44 PM GMT

PDB ID	:	4ACA
Title	:	CRYSTAL STRUCTURE OF TRANSLATION ELONGATION FACTOR SELB FROM METHANOCOCCUS MARIPALUDIS, APO FORM
Authors	:	Leibundgut, M.; Frick, C.; Thanbichler, M.; Boeck, A.; Ban, N.
Deposited on	:	2011-12-14
Resolution	:	3.15 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:

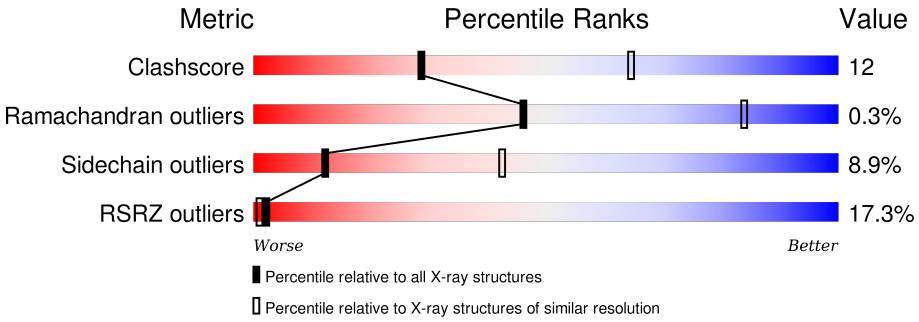
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.15 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))
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	16% 63% 27% • 7%
1	B	482	15% 65% 27% • 5%
1	C	482	5% 73% 22% • •
1	D	482	30% 65% 28% • •

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
1	CMH	A	340	-	-	X	-
1	CMH	B	371	-	-	X	-
2	SO4	B	1472	-	-	-	X
4	5GP	B	1474	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14529 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	448	Total	C	Hg	N	O	S	0	0	0
			3475	2220	4	593	644	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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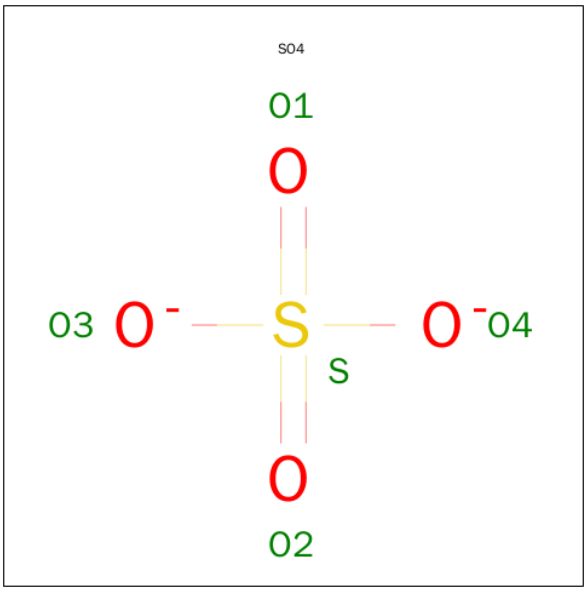
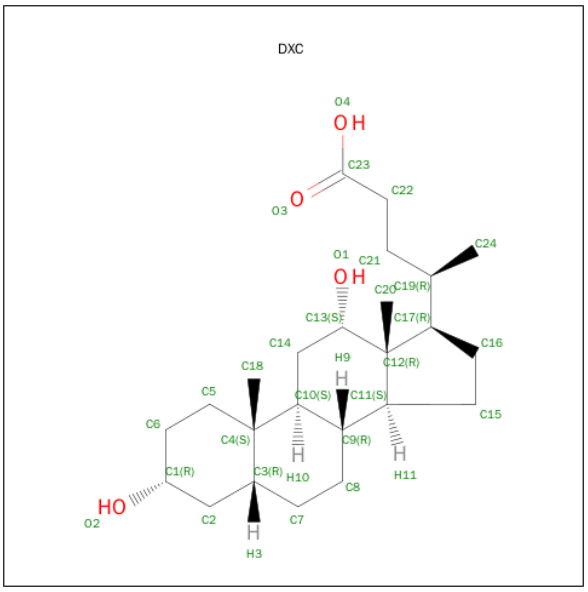
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	SER	-	EXPRESSION TAG	UNP Q8J307
B	-5	ILE	-	EXPRESSION TAG	UNP Q8J307
B	-4	GLU	-	EXPRESSION TAG	UNP Q8J307
B	-3	GLY	-	EXPRESSION TAG	UNP Q8J307
B	-2	ARG	-	EXPRESSION TAG	UNP Q8J307
B	-1	PRO	-	EXPRESSION TAG	UNP Q8J307
B	0	HIS	-	EXPRESSION TAG	UNP Q8J307
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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



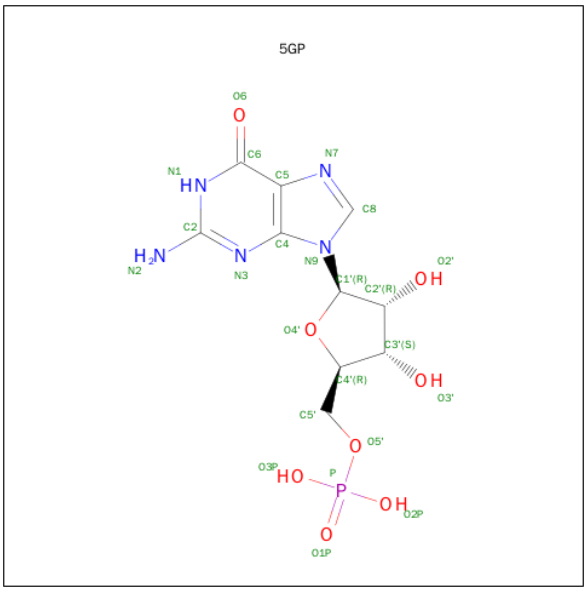
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 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
3	B	1	Total C O 28 24 4	0	0
3	C	1	Total C O 28 24 4	0	0
3	C	1	Total C O 28 24 4	0	0
3	C	1	Total C O 28 24 4	0	0
3	C	1	Total C O 28 24 4	0	0
3	C	1	Total C O 28 24 4	0	0
3	C	1	Total C O 28 24 4	0	0

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



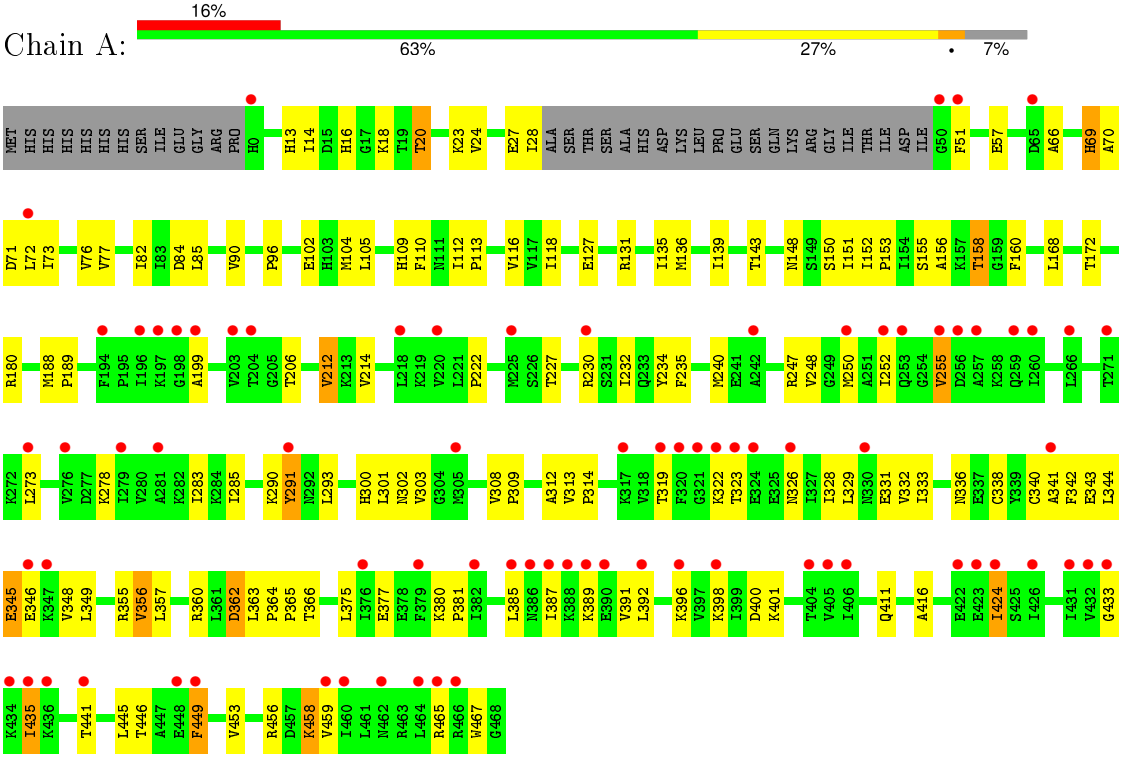
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	24	10	5	8	1	0	0

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.

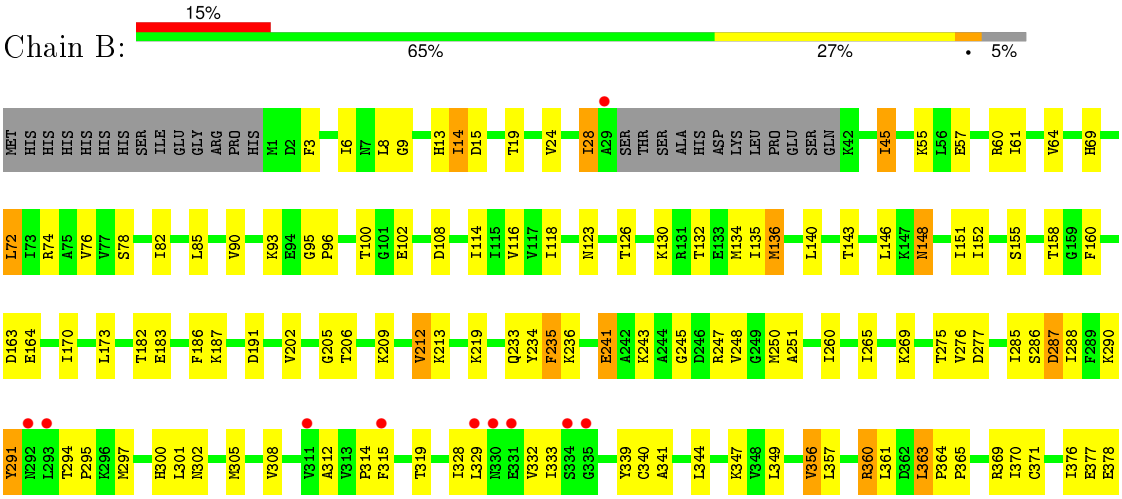
- Molecule 1: TRANSLATION ELONGATION FACTOR SELB

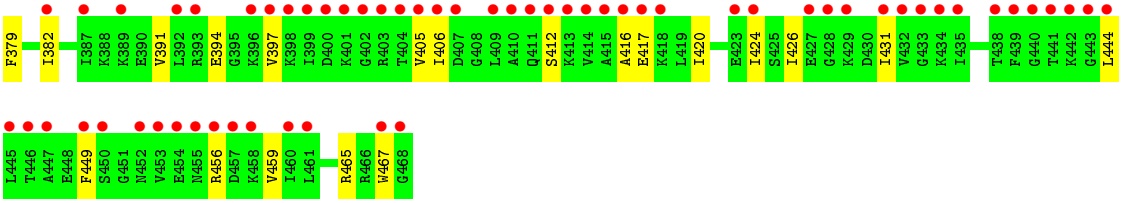
Chain A:



- Molecule 1: TRANSLATION ELONGATION FACTOR SELB

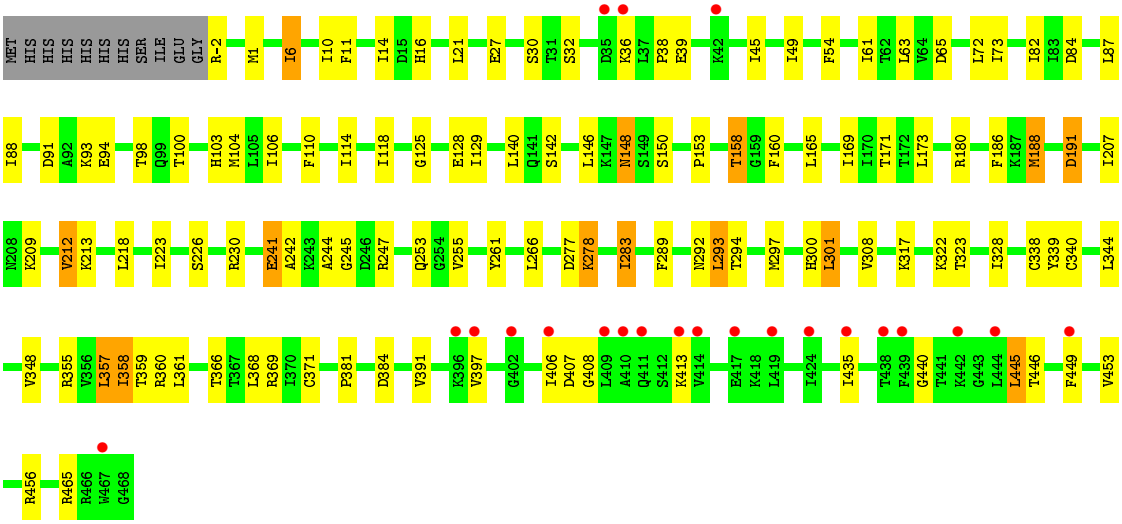
Chain B:





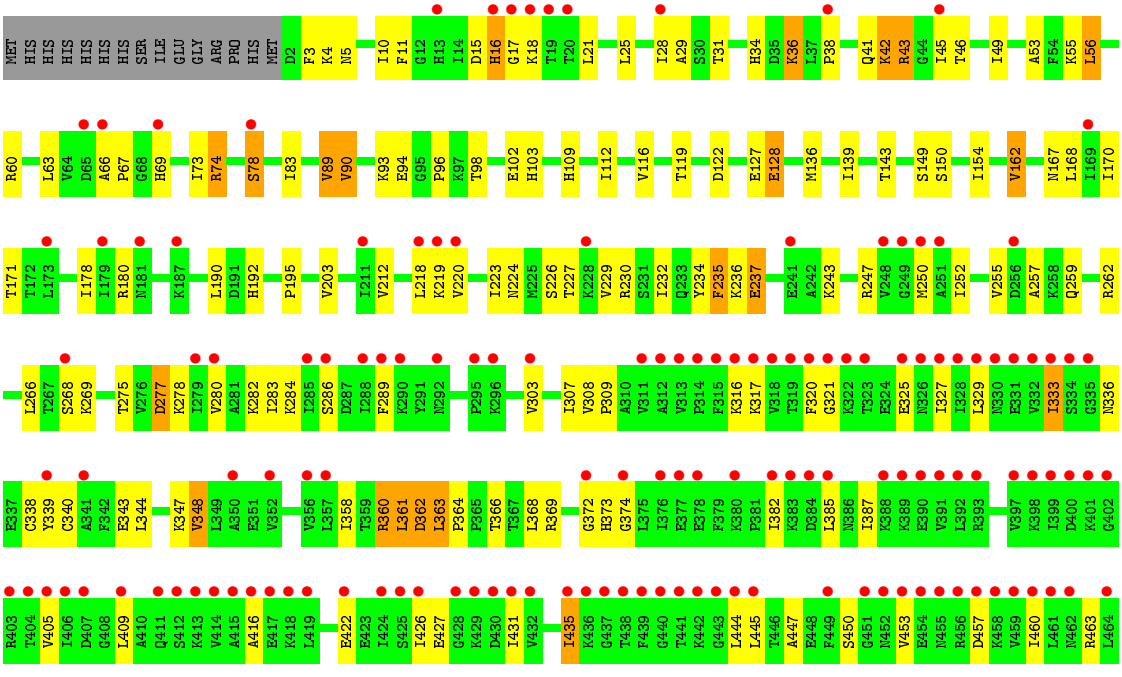
• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

Chain C:



• Molecule 1: TRANSLATION ELONGATION FACTOR SELB

Chain D:




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	146.86Å 146.86Å 297.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.15 48.07 – 3.15	Depositor EDS
% Data completeness (in resolution range)	86.9 (19.97-3.15) 90.3 (48.07-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.172 , 0.215 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	100.6	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 126.3	EDS
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 63646 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: 5GP, DXC, SO4, CMH

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	0/3484	0.54	0/4684
1	B	0.34	0/3541	0.57	0/4760
1	C	0.39	0/3664	0.62	0/4929
1	D	0.29	0/3626	0.52	0/4878
All	All	0.33	0/14315	0.56	0/19251

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	3475	0	3656	83	0
1	B	3533	0	3728	91	0
1	C	3651	0	3838	70	0
1	D	3615	0	3799	101	0
2	B	10	0	0	1	0
2	C	25	0	0	1	0
3	B	28	0	39	2	0
3	C	168	0	234	11	0
4	B	24	0	12	2	0
All	All	14529	0	15306	343	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 (343) 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:D:283:ILE:HG13	1:D:340:CMH:HB3	1.21	1.15
1:C:338:CMH:HB3	1:C:340:CMH:CM	2.03	0.86
1:D:223:ILE:HG21	1:D:259:GLN:HB3	1.58	0.85
1:D:284:LYS:HG3	1:D:336:ASN:HB2	1.63	0.81
1:D:416:ALA:HB1	1:D:445:LEU:HD21	1.61	0.79
1:C:283:ILE:HG12	1:C:358:ILE:HD11	1.70	0.74
1:C:6:ILE:HD12	1:C:173:LEU:HD13	1.71	0.73
1:B:360:ARG:NH1	1:B:371:CMH:SG	2.61	0.73
1:D:116:VAL:HG11	1:D:136:MET:HG2	1.69	0.72
1:B:158:THR:HG23	1:D:363:LEU:HB3	1.75	0.69
1:D:422:GLU:H	1:D:435:ILE:HG22	1.57	0.69
1:B:302:ASN:HB2	1:B:357:LEU:HB3	1.76	0.68
1:C:158:THR:HG22	1:C:160:PHE:H	1.58	0.68
1:D:21:LEU:HD22	1:D:89:VAL:HG11	1.76	0.67
1:D:427:GLU:HG2	1:D:460:ILE:HG13	1.76	0.67
1:B:82:ILE:HG23	1:B:245:GLY:HA2	1.76	0.67
1:C:283:ILE:HD13	1:C:340:CMH:HB3	1.74	0.67
1:B:233:GLN:HE21	1:B:236:LYS:HA	1.59	0.67
1:C:308:VAL:HG21	1:C:344:LEU:HD13	1.77	0.66
1:D:277:ASP:HB3	1:D:347:LYS:HE2	1.77	0.66
1:A:234:TYR:HB2	1:A:248:VAL:HG12	1.77	0.66
1:A:152:ILE:HD11	1:A:168:LEU:HD22	1.80	0.64
1:D:360:ARG:HD2	1:D:363:LEU:HD11	1.78	0.64
1:D:316:LYS:N	1:D:327:ILE:O	2.29	0.64
1:D:67:PRO:HA	1:D:78:SER:HB2	1.78	0.64
1:B:143:THR:HG21	1:B:146:LEU:HB2	1.80	0.63
1:B:361:LEU:HA	1:B:369:ARG:HD2	1.81	0.63
1:A:118:ILE:HB	1:A:153:PRO:HA	1.81	0.63
1:B:288:ILE:HB	4:B:1474:5GP:HN22	1.64	0.62
1:D:4:LYS:NZ	1:D:178:ILE:O	2.31	0.62
1:C:82:ILE:HG23	1:C:245:GLY:HA2	1.80	0.62
1:B:132:THR:HA	1:B:135:ILE:HD12	1.81	0.62
1:B:69:HIS:NE2	1:B:102:GLU:OE1	2.25	0.62
1:D:218:LEU:HD11	1:D:229:VAL:HG22	1.81	0.61
1:D:73:ILE:O	1:D:74:ARG:HG3	2.00	0.61
1:A:435:ILE:HD11	1:A:445:LEU:HD22	1.83	0.60
1:D:43:ARG:HB3	1:D:45:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:HA3	1:A:449:PHE:HB3	1.82	0.60
1:C:88:ILE:HD12	1:C:114:ILE:HD13	1.83	0.59
1:C:88:ILE:HD13	1:C:104:MET:HG2	1.83	0.59
1:B:116:VAL:HB	1:B:151:ILE:HG12	1.85	0.59
1:B:74:ARG:NH2	2:B:1471:SO4:O4	2.35	0.59
1:D:109:HIS:CG	1:D:373:HIS:HE1	2.21	0.58
1:D:93:LYS:HA	1:D:128:GLU:HG2	1.84	0.58
1:D:338:CMH:SG	1:D:339:TYR:N	2.75	0.58
1:B:114:ILE:HG12	1:B:146:LEU:HD22	1.86	0.58
1:C:110:PHE:CD2	1:C:355:ARG:HD2	2.37	0.58
1:D:409:LEU:HD12	1:D:445:LEU:HD12	1.85	0.58
1:C:27:GLU:HB3	1:C:32:SER:HB2	1.84	0.58
1:B:426:ILE:HB	1:B:431:ILE:HG23	1.85	0.58
1:D:360:ARG:HH11	1:D:363:LEU:HD21	1.67	0.57
1:A:362:ASP:N	1:A:362:ASP:OD1	2.32	0.57
1:B:213:LYS:HG2	1:B:241:GLU:HB2	1.86	0.57
1:C:191:ASP:OD2	1:C:247:ARG:NH1	2.31	0.57
1:B:90:VAL:HG13	1:B:118:ILE:HG12	1.87	0.57
1:C:188:MET:HG3	1:C:207:ILE:HG12	1.86	0.57
1:C:11:PHE:HB3	1:C:103:HIS:ND1	2.20	0.57
1:D:109:HIS:HB3	1:D:373:HIS:HE1	1.70	0.57
1:D:29:ALA:HB2	1:D:56:LEU:HG	1.86	0.57
1:D:83:ILE:HG22	1:D:112:ILE:HD13	1.86	0.57
1:A:96:PRO:HB3	1:A:136:MET:HE1	1.86	0.57
1:C:125:GLY:O	1:C:129:ILE:HG13	2.05	0.57
1:C:106:ILE:HG12	1:C:357:LEU:HD21	1.87	0.56
1:D:232:ILE:HG12	1:D:250:MET:HG2	1.87	0.56
1:D:38:PRO:HB3	1:D:42:LYS:HD2	1.88	0.56
1:A:158:THR:HG22	1:A:160:PHE:H	1.69	0.56
1:C:100:THR:O	1:C:104:MET:HG3	2.06	0.56
1:C:36:LYS:HE3	1:C:38:PRO:HB3	1.87	0.56
1:A:66:ALA:HB1	1:A:71:ASP:HB3	1.88	0.56
1:D:109:HIS:CG	1:D:373:HIS:CE1	2.94	0.56
1:D:96:PRO:HG3	1:D:136:MET:SD	2.46	0.56
1:A:278:LYS:HD2	1:A:343:GLU:HG2	1.88	0.56
1:D:36:LYS:HB3	1:D:236:LYS:HD2	1.88	0.55
1:B:187:LYS:HB3	1:B:209:LYS:HG3	1.89	0.55
1:B:72:LEU:O	1:B:76:VAL:HG23	2.06	0.55
1:A:313:VAL:HG23	1:A:341:ALA:HB3	1.88	0.55
1:C:283:ILE:HG21	1:C:371:CMH:CM	2.36	0.55
1:A:345:GLU:HG2	1:A:346:GLU:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PHE:CE2	1:C:72:LEU:HD22	2.42	0.55
1:A:24:VAL:HG21	1:A:156:ALA:HB1	1.89	0.54
1:C:165:LEU:O	1:C:169:ILE:HG13	2.08	0.54
1:D:74:ARG:HG2	1:D:361:LEU:HD13	1.88	0.54
1:B:8:LEU:HD12	1:B:85:LEU:O	2.08	0.54
1:D:102:GLU:HB2	1:D:366:THR:HG22	1.89	0.54
1:C:148:ASN:OD1	1:C:148:ASN:N	2.41	0.54
1:B:287:ASP:OD1	1:B:287:ASP:N	2.36	0.53
1:A:77:VAL:HG11	1:A:302:ASN:HB3	1.90	0.53
1:B:6:ILE:HG22	1:B:61:ILE:HG23	1.89	0.53
1:D:358:ILE:HD12	1:D:372:GLY:HA3	1.90	0.53
1:A:240:MET:HE1	1:B:95:GLY:HA3	1.91	0.53
1:C:397:VAL:HG11	1:C:453:VAL:HG23	1.90	0.53
1:A:283:ILE:HD12	1:A:340:CMH:HB3	1.91	0.53
1:A:14:ILE:HA	1:A:18:LYS:NZ	2.23	0.53
1:C:118:ILE:HB	1:C:153:PRO:HA	1.90	0.53
1:A:293:LEU:HD13	1:A:329:LEU:HD23	1.91	0.53
1:B:82:ILE:HD13	1:B:206:THR:HG22	1.91	0.52
1:B:363:LEU:HD13	1:B:364:PRO:HD2	1.91	0.52
1:B:155:SER:HB3	1:B:160:PHE:HB3	1.91	0.52
1:A:110:PHE:HD1	1:A:355:ARG:HD2	1.73	0.52
1:C:110:PHE:CE2	1:C:355:ARG:HD2	2.44	0.52
1:D:3:PHE:HE2	1:D:55:LYS:HE3	1.74	0.52
1:B:406:ILE:HD11	1:B:449:PHE:HZ	1.75	0.52
1:C:27:GLU:HA	1:C:30:SER:HB3	1.92	0.51
1:B:93:LYS:HE3	1:B:123:ASN:O	2.09	0.51
1:C:293:LEU:HD22	1:C:371:CMH:CM	2.40	0.51
1:D:34:HIS:CD2	1:D:236:LYS:HB2	2.45	0.51
1:A:389:LYS:HB3	1:A:465:ARG:HB3	1.92	0.51
1:D:69:HIS:CE1	1:D:103:HIS:CE1	2.98	0.51
1:D:90:VAL:HG21	1:D:136:MET:HE1	1.93	0.51
1:A:136:MET:HE2	1:A:139:ILE:HD12	1.93	0.51
1:A:300:HIS:CE1	1:A:309:PRO:HG3	2.46	0.51
1:D:282:LYS:O	1:D:374:GLY:HA2	2.11	0.51
1:D:435:ILE:HG13	1:D:447:ALA:HB2	1.93	0.50
1:C:317:LYS:HD2	1:C:339:TYR:CE2	2.46	0.50
1:B:143:THR:HG22	1:B:146:LEU:H	1.75	0.50
1:B:329:LEU:HB3	1:B:332:VAL:HB	1.93	0.50
1:D:463:ARG:HE	1:D:465:ARG:CZ	2.25	0.50
1:B:60:ARG:HD3	1:B:235:PHE:CD2	2.47	0.50
1:B:265:ILE:HG13	1:B:349:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ASP:HA	1:D:18:LYS:HE2	1.92	0.50
1:A:336:ASN:HA	1:A:338:CMH:CM	2.42	0.49
1:B:152:ILE:HD11	1:B:164:GLU:HB2	1.94	0.49
1:A:285:ILE:HG12	1:A:291:TYR:CE2	2.47	0.49
1:C:213:LYS:HG2	1:C:241:GLU:HB2	1.94	0.49
1:B:251:ALA:HB1	1:C:1:MET:HE1	1.94	0.49
1:B:140:LEU:O	1:B:143:THR:HB	2.11	0.49
1:A:70:ALA:HA	1:A:73:ILE:HD12	1.92	0.49
1:A:387:ILE:HG23	1:A:467:TRP:HB3	1.95	0.49
1:D:109:HIS:CB	1:D:373:HIS:HE1	2.26	0.49
1:A:398:LYS:HE2	1:A:456:ARG:NH1	2.28	0.49
1:A:110:PHE:HE1	1:A:355:ARG:HB3	1.77	0.49
1:A:285:ILE:HG23	1:A:291:TYR:CD2	2.48	0.49
1:A:131:ARG:O	1:A:135:ILE:HG13	2.11	0.49
1:B:148:ASN:ND2	1:D:127:GLU:HB3	2.27	0.49
1:B:294:THR:HB	1:B:297:MET:HB3	1.94	0.49
1:D:56:LEU:HD22	1:D:170:ILE:HD11	1.94	0.49
1:B:377:GLU:HG2	1:B:378:GLU:HG3	1.95	0.49
1:A:338:CMH:HB2	1:A:340:CMH:CM	2.43	0.49
1:D:34:HIS:N	1:D:53:ALA:O	2.46	0.48
1:D:303:VAL:HB	1:D:348:VAL:HG11	1.94	0.48
1:D:360:ARG:HD3	1:D:362:ASP:HB2	1.94	0.48
1:C:322:LYS:HG3	1:C:323:THR:H	1.78	0.48
1:B:243:LYS:HB3	1:B:243:LYS:HE2	1.62	0.48
1:C:10:ILE:HD13	1:C:87:LEU:HB2	1.95	0.48
1:B:301:LEU:HD11	1:B:356:VAL:HG13	1.96	0.48
1:B:160:PHE:CZ	1:D:98:THR:HG23	2.48	0.48
1:D:405:VAL:CG1	1:D:444:LEU:HB3	2.44	0.48
1:D:405:VAL:HG11	1:D:444:LEU:HB3	1.95	0.48
1:B:134:MET:SD	1:D:94:GLU:HG2	2.53	0.48
1:B:285:ILE:HD12	1:B:371:CMH:CM	2.44	0.48
1:A:360:ARG:HG2	1:A:363:LEU:HG	1.96	0.48
1:B:82:ILE:HG21	1:B:206:THR:HG21	1.96	0.48
1:B:186:PHE:CE1	1:B:212:VAL:HG22	2.49	0.48
1:A:308:VAL:HG21	1:A:344:LEU:HD13	1.95	0.48
1:A:355:ARG:HG2	1:A:375:LEU:HD23	1.96	0.47
1:D:167:ASN:O	1:D:171:THR:OG1	2.22	0.47
1:B:405:VAL:HG11	1:B:444:LEU:HD13	1.96	0.47
1:A:155:SER:OG	1:A:158:THR:HB	2.14	0.47
1:C:-2:ARG:HE	3:C:1476:DXC:H21	1.79	0.47
1:C:16:HIS:NE2	1:C:94:GLU:OE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LYS:HG2	1:D:343:GLU:HG2	1.96	0.47
1:D:43:ARG:HH12	1:D:230:ARG:HB3	1.78	0.47
1:A:110:PHE:CD1	1:A:355:ARG:HD2	2.50	0.47
1:A:301:LEU:HD11	1:A:356:VAL:HG13	1.95	0.47
1:A:424:ILE:HG13	1:A:459:VAL:HG13	1.97	0.47
1:D:5:ASN:OD1	1:D:234:TYR:OH	2.24	0.47
1:B:78:SER:HB2	1:B:305:MET:HG2	1.96	0.47
1:D:34:HIS:NE2	1:D:235:PHE:O	2.47	0.47
1:D:5:ASN:HD22	1:D:243:LYS:HE3	1.80	0.47
1:B:276:VAL:HG11	1:B:379:PHE:CD1	2.49	0.47
1:B:277:ASP:HB2	1:B:347:LYS:HE3	1.96	0.47
1:A:105:LEU:O	1:A:109:HIS:ND1	2.42	0.47
1:A:212:VAL:HG11	1:A:250:MET:HE1	1.96	0.46
1:D:42:LYS:HE2	1:D:237:GLU:HA	1.97	0.46
1:D:28:ILE:HG22	1:D:162:VAL:HG13	1.98	0.46
1:A:312:ALA:HB1	1:A:340:CMH:SG	2.55	0.46
1:D:17:GLY:HA2	1:D:119:THR:HG21	1.97	0.46
1:B:3:PHE:CE1	1:B:55:LYS:HE3	2.51	0.46
1:A:456:ARG:O	1:A:458:LYS:NZ	2.30	0.46
1:D:190:LEU:HG	1:D:203:VAL:HB	1.97	0.46
1:D:218:LEU:HD13	1:D:266:LEU:HD11	1.97	0.46
1:A:449:PHE:CD1	1:A:453:VAL:HG21	2.50	0.46
1:B:9:GLY:HA2	1:B:64:VAL:HB	1.98	0.46
1:D:122:ASP:N	1:D:122:ASP:OD1	2.48	0.46
1:C:54:PHE:HE1	1:C:63:LEU:HD21	1.80	0.46
1:B:285:ILE:HD13	1:B:291:TYR:HB3	1.96	0.46
1:A:230:ARG:NH2	4:B:1474:5GP:O2'	2.49	0.46
1:C:27:GLU:O	1:C:32:SER:N	2.48	0.46
1:A:326:ASN:HD22	1:A:385:LEU:HB3	1.80	0.46
1:A:240:MET:CE	1:B:96:PRO:HD2	2.46	0.45
1:D:268:SER:OG	1:D:269:LYS:N	2.49	0.45
1:B:424:ILE:HD12	1:B:459:VAL:HG11	1.99	0.45
1:B:285:ILE:HG13	1:B:371:CMH:O	2.15	0.45
1:A:20:THR:O	1:A:24:VAL:HG23	2.16	0.45
1:C:300:HIS:ND1	1:C:361:LEU:HD12	2.32	0.45
1:A:340:CMH:HB2	1:A:342:PHE:CE2	2.51	0.45
1:C:435:ILE:HD12	1:C:445:LEU:HD13	1.98	0.45
1:A:85:LEU:HD13	1:A:172:THR:HG21	1.98	0.45
1:D:219:LYS:HE3	1:D:224:ASN:OD1	2.16	0.45
1:C:186:PHE:CE1	1:C:212:VAL:HG22	2.52	0.45
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:PRO:HG3	1:D:136:MET:CE	2.47	0.45
1:D:74:ARG:O	1:D:307:ILE:HB	2.17	0.45
1:A:227:THR:HG21	1:A:255:VAL:HG22	1.99	0.45
1:B:202:VAL:HA	1:B:250:MET:O	2.16	0.45
1:B:341:ALA:HB1	1:B:382:ILE:HG12	1.99	0.45
1:D:212:VAL:HG22	1:D:232:ILE:HD11	1.99	0.44
1:A:222:PRO:HB3	1:A:349:LEU:HD21	2.00	0.44
1:B:251:ALA:HB1	1:C:1:MET:CE	2.47	0.44
1:C:140:LEU:HD22	1:C:146:LEU:O	2.17	0.44
1:B:191:ASP:OD2	1:B:247:ARG:NH1	2.47	0.44
1:D:227:THR:HG21	1:D:252:ILE:HD12	1.99	0.44
1:C:93:LYS:HG3	1:C:128:GLU:OE1	2.17	0.44
1:C:407:ASP:OD1	1:C:408:GLY:N	2.50	0.44
1:D:363:LEU:HA	1:D:364:PRO:HD3	1.66	0.44
1:D:10:ILE:HD11	1:D:63:LEU:HD11	2.00	0.44
1:B:397:VAL:O	1:B:456:ARG:N	2.47	0.44
1:B:234:TYR:HB2	1:B:248:VAL:HG12	2.00	0.44
1:A:199:ALA:HB3	1:B:290:LYS:HD2	1.99	0.44
1:A:290:LYS:HA	1:A:290:LYS:HD3	1.75	0.44
1:B:315:PHE:O	1:B:339:TYR:N	2.50	0.44
1:B:130:LYS:HA	1:B:130:LYS:HD2	1.77	0.44
1:A:72:LEU:O	1:A:76:VAL:HG23	2.16	0.44
1:C:158:THR:HG21	3:C:1478:DXC:O2	2.17	0.44
1:A:136:MET:CE	1:A:139:ILE:HD12	2.48	0.44
1:A:84:ASP:OD2	1:A:180:ARG:NH2	2.51	0.44
3:C:1479:DXC:H222	3:C:1479:DXC:H243	1.77	0.44
1:D:283:ILE:HA	1:D:373:HIS:O	2.18	0.44
1:B:314:PRO:HA	1:B:339:TYR:O	2.18	0.44
1:D:426:ILE:HB	1:D:431:ILE:HG12	1.98	0.44
1:B:364:PRO:HA	1:B:365:PRO:HD3	1.79	0.44
1:C:10:ILE:HD11	1:C:87:LEU:HD12	2.00	0.44
1:C:10:ILE:HD12	1:C:21:LEU:HD23	1.99	0.44
1:B:82:ILE:HG21	1:B:206:THR:CG2	2.48	0.43
1:D:329:LEU:HD22	1:D:338:CMH:CB	2.48	0.43
1:C:39:GLU:H	1:C:39:GLU:HG2	1.63	0.43
1:C:406:ILE:HD11	1:C:449:PHE:CZ	2.52	0.43
1:D:74:ARG:HH22	1:D:309:PRO:HD3	1.83	0.43
1:C:1:MET:HB2	3:C:1476:DXC:H62	1.99	0.43
1:A:23:LYS:O	1:A:27:GLU:HG2	2.19	0.43
1:B:391:VAL:HB	1:B:465:ARG:HD3	2.00	0.43
1:A:400:ASP:OD1	1:A:401:LYS:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LYS:HE2	1:D:339:TYR:OH	2.18	0.43
1:D:15:ASP:OD1	1:D:16:HIS:ND1	2.51	0.43
1:B:417:GLU:O	1:B:420:ILE:HG12	2.18	0.43
1:C:301:LEU:CD1	1:C:358:ILE:HG23	2.48	0.43
1:D:5:ASN:OD1	1:D:60:ARG:HD3	2.18	0.43
1:A:116:VAL:HB	1:A:151:ILE:HG12	2.00	0.43
1:B:24:VAL:O	1:B:28:ILE:HG22	2.18	0.43
1:B:360:ARG:HH12	1:B:371:CMH:CB	2.31	0.43
1:B:96:PRO:HG3	1:B:136:MET:SD	2.58	0.43
1:B:416:ALA:O	1:B:420:ILE:HG23	2.19	0.43
1:B:6:ILE:HG12	1:B:173:LEU:HD13	2.00	0.43
1:A:391:VAL:HG21	1:A:465:ARG:HD3	2.01	0.43
1:B:130:LYS:HE3	1:B:134:MET:HE3	2.01	0.43
1:D:308:VAL:HG21	1:D:344:LEU:HB3	2.00	0.43
1:A:51:PHE:CE2	1:A:247:ARG:HG2	2.53	0.43
1:C:188:MET:HE3	1:C:188:MET:HB3	1.93	0.43
1:A:240:MET:CE	1:B:95:GLY:HA3	2.49	0.43
1:C:406:ILE:HD11	1:C:449:PHE:HZ	1.83	0.43
1:B:57:GLU:HG3	1:B:170:ILE:HD13	2.00	0.43
1:C:465:ARG:HG2	2:C:1473:SO4:O1	2.19	0.43
1:A:314:PRO:O	1:A:328:ILE:HD12	2.19	0.43
1:A:84:ASP:O	1:A:113:PRO:HG2	2.19	0.42
1:D:431:ILE:HB	1:D:450:SER:O	2.19	0.42
1:B:13:HIS:H	1:B:100:THR:HG22	1.84	0.42
1:A:13:HIS:O	1:A:16:HIS:HB2	2.19	0.42
1:B:219:LYS:HE2	1:B:269:LYS:HA	2.01	0.42
1:C:230:ARG:HD2	1:C:253:GLN:CD	2.40	0.42
1:D:21:LEU:O	1:D:25:LEU:HB2	2.19	0.42
1:B:191:ASP:OD2	1:B:205:GLY:HA2	2.20	0.42
1:D:192:HIS:HA	1:D:262:ARG:HD2	2.02	0.42
1:C:91:ASP:HB3	1:C:94:GLU:HG2	2.02	0.42
1:D:247:ARG:HD2	1:D:247:ARG:HA	1.77	0.42
1:D:363:LEU:HD13	1:D:369:ARG:HH11	1.84	0.42
1:C:357:LEU:HA	1:C:357:LEU:HD12	1.82	0.42
1:A:329:LEU:C	1:A:331:GLU:H	2.22	0.42
1:D:66:ALA:HB1	1:D:69:HIS:ND1	2.35	0.42
1:C:277:ASP:HB3	1:C:278:LYS:HG2	2.01	0.42
1:D:280:VAL:HG21	1:D:385:LEU:HD21	2.01	0.42
1:A:158:THR:HG22	1:A:160:PHE:N	2.35	0.42
1:A:214:VAL:HG22	1:A:232:ILE:HG13	2.01	0.42
3:C:1478:DXC:H22	3:C:1478:DXC:H82	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ILE:H	1:D:73:ILE:HG13	1.58	0.42
1:A:109:HIS:HD1	1:A:109:HIS:H	1.68	0.42
1:A:69:HIS:CD2	1:A:70:ALA:H	2.38	0.42
1:D:218:LEU:CD1	1:D:229:VAL:HG22	2.50	0.41
1:A:302:ASN:HB2	1:A:357:LEU:HB3	2.02	0.41
1:A:112:ILE:HA	1:A:113:PRO:HD2	1.90	0.41
3:C:1479:DXC:H71	3:C:1479:DXC:H182	1.86	0.41
1:D:320:PHE:HE1	1:D:325:GLU:HG3	1.85	0.41
1:A:380:LYS:HA	1:A:381:PRO:HD3	1.90	0.41
1:A:322:LYS:HG3	1:A:323:THR:H	1.85	0.41
1:B:291:TYR:HD1	1:B:333:ILE:HG22	1.85	0.41
1:D:150:SER:OG	1:D:168:LEU:HD21	2.20	0.41
1:C:360:ARG:O	1:C:369:ARG:HB3	2.19	0.41
3:B:1473:DXC:H13	3:B:1473:DXC:H242	2.02	0.41
1:B:108:ASP:CG	1:B:143:THR:HG23	2.41	0.41
1:C:218:LEU:HD12	1:C:266:LEU:HD21	2.02	0.41
1:D:11:PHE:CZ	1:D:67:PRO:HD2	2.55	0.41
1:D:43:ARG:HH22	1:D:230:ARG:HD3	1.85	0.41
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.86	0.41
1:B:234:TYR:CD2	1:B:235:PHE:HB2	2.55	0.41
1:B:14:ILE:O	1:B:15:ASP:HB2	2.20	0.41
1:C:49:ILE:HD11	3:C:1475:DXC:H161	2.03	0.41
1:C:381:PRO:HD2	1:C:384:ASP:HB2	2.03	0.41
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.76	0.41
1:A:206:THR:HA	1:A:247:ARG:HA	2.03	0.41
1:B:312:ALA:HB1	1:B:340:CMH:SG	2.61	0.41
1:A:188:MET:HA	1:A:189:PRO:HD3	1.92	0.41
1:B:328:ILE:HG21	1:B:467:TRP:CD1	2.56	0.41
1:C:84:ASP:CG	1:C:180:ARG:HH22	2.23	0.41
1:D:10:ILE:HD13	1:D:21:LEU:HD23	2.02	0.41
1:C:1:MET:HB2	3:C:1476:DXC:C6	2.51	0.41
1:A:364:PRO:HA	1:A:365:PRO:HD3	1.92	0.41
1:D:3:PHE:CE2	1:D:55:LYS:HE3	2.54	0.41
3:C:1480:DXC:H243	3:C:1480:DXC:H221	1.70	0.41
1:C:289:PHE:CZ	1:C:371:CMH:HB2	2.56	0.41
1:C:27:GLU:C	1:C:32:SER:HB2	2.41	0.41
1:A:158:THR:CG2	1:A:160:PHE:HB2	2.51	0.41
1:A:303:VAL:HG22	1:A:356:VAL:HG22	2.03	0.41
3:C:1479:DXC:H203	3:C:1479:DXC:H19	1.81	0.41
3:B:1473:DXC:H61	3:B:1473:DXC:H10	1.83	0.41
1:D:218:LEU:HD13	1:D:266:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:HIS:HB3	1:D:53:ALA:HB3	2.02	0.41
1:B:305:MET:HB3	1:B:305:MET:HE3	1.93	0.40
1:D:227:THR:HB	1:D:255:VAL:HG23	2.03	0.40
1:D:5:ASN:O	1:D:180:ARG:NH2	2.49	0.40
1:B:295:PRO:HB3	1:B:328:ILE:HD11	2.01	0.40
1:C:413:LYS:HB2	1:C:440:GLY:O	2.22	0.40
1:D:74:ARG:HH11	1:D:307:ILE:HG22	1.86	0.40
1:B:376:ILE:HG21	1:B:379:PHE:CE1	2.56	0.40
1:B:45:ILE:HG12	1:B:45:ILE:O	2.21	0.40
1:D:195:PRO:HD3	1:D:257:ALA:HB1	2.03	0.40
1:B:114:ILE:HD13	1:B:146:LEU:HD13	2.03	0.40
1:B:78:SER:CB	1:B:305:MET:HG2	2.52	0.40
1:D:223:ILE:HD13	1:D:259:GLN:HB3	2.02	0.40
1:C:158:THR:HG22	1:C:160:PHE:N	2.33	0.40
1:A:416:ALA:HB1	1:A:445:LEU:HD21	2.04	0.40
1:A:158:THR:HG22	1:A:160:PHE:HB2	2.02	0.40
1:C:212:VAL:HG23	1:C:242:ALA:HB3	2.04	0.40
3:C:1475:DXC:H221	3:C:1475:DXC:H243	1.73	0.40
1:C:209:LYS:HA	1:C:244:ALA:HB2	2.02	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	440/482 (91%)	420 (96%)	19 (4%)	1 (0%)	52 88
1	B	448/482 (93%)	430 (96%)	18 (4%)	0	100 100
1	C	465/482 (96%)	439 (94%)	26 (6%)	0	100 100
1	D	461/482 (96%)	433 (94%)	24 (5%)	4 (1%)	21 65
All	All	1814/1928 (94%)	1722 (95%)	87 (5%)	5 (0%)	46 84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	LYS
1	A	69	HIS
1	D	333	ILE
1	D	321	GLY
1	D	382	ILE

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	382/412 (93%)	346 (91%)	36 (9%)	11	39
1	B	388/412 (94%)	359 (92%)	29 (8%)	17	53
1	C	402/412 (98%)	364 (90%)	38 (10%)	11	38
1	D	398/412 (97%)	361 (91%)	37 (9%)	11	40
All	All	1570/1648 (95%)	1430 (91%)	140 (9%)	12	42

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	28	ILE
1	A	57	GLU
1	A	82	ILE
1	A	90	VAL
1	A	102	GLU
1	A	104	MET
1	A	127	GLU
1	A	143	THR
1	A	148	ASN
1	A	150	SER
1	A	158	THR
1	A	212	VAL
1	A	235	PHE
1	A	252	ILE

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Mol	Chain	Res	Type
1	A	255	VAL
1	A	273	LEU
1	A	291	TYR
1	A	319	THR
1	A	332	VAL
1	A	333	ILE
1	A	345	GLU
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	396	LYS
1	A	411	GLN
1	A	424	ILE
1	A	435	ILE
1	A	441	THR
1	A	446	THR
1	A	449	PHE
1	A	458	LYS
1	B	14	ILE
1	B	19	THR
1	B	28	ILE
1	B	45	ILE
1	B	72	LEU
1	B	126	THR
1	B	136	MET
1	B	148	ASN
1	B	163	ASP
1	B	182	THR
1	B	183	GLU
1	B	212	VAL
1	B	235	PHE
1	B	241	GLU
1	B	260	ILE
1	B	275	THR
1	B	286	SER
1	B	287	ASP
1	B	291	TYR
1	B	300	HIS
1	B	308	VAL

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Mol	Chain	Res	Type
1	B	319	THR
1	B	344	LEU
1	B	356	VAL
1	B	360	ARG
1	B	363	LEU
1	B	370	ILE
1	B	394	GLU
1	B	412	SER
1	C	6	ILE
1	C	14	ILE
1	C	45	ILE
1	C	61	ILE
1	C	65	ASP
1	C	73	ILE
1	C	98	THR
1	C	142	SER
1	C	148	ASN
1	C	150	SER
1	C	158	THR
1	C	171	THR
1	C	188	MET
1	C	191	ASP
1	C	212	VAL
1	C	223	ILE
1	C	226	SER
1	C	241	GLU
1	C	255	VAL
1	C	261	TYR
1	C	278	LYS
1	C	283	ILE
1	C	292	ASN
1	C	293	LEU
1	C	294	THR
1	C	297	MET
1	C	301	LEU
1	C	328	ILE
1	C	348	VAL
1	C	357	LEU
1	C	358	ILE
1	C	359	THR
1	C	366	THR
1	C	368	LEU

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Mol	Chain	Res	Type
1	C	391	VAL
1	C	445	LEU
1	C	446	THR
1	C	456	ARG
1	D	16	HIS
1	D	31	THR
1	D	36	LYS
1	D	41	GLN
1	D	43	ARG
1	D	46	THR
1	D	49	ILE
1	D	56	LEU
1	D	74	ARG
1	D	78	SER
1	D	89	VAL
1	D	90	VAL
1	D	128	GLU
1	D	139	ILE
1	D	143	THR
1	D	149	SER
1	D	154	ILE
1	D	162	VAL
1	D	220	VAL
1	D	226	SER
1	D	235	PHE
1	D	237	GLU
1	D	275	THR
1	D	277	ASP
1	D	286	SER
1	D	289	PHE
1	D	333	ILE
1	D	348	VAL
1	D	360	ARG
1	D	361	LEU
1	D	362	ASP
1	D	363	LEU
1	D	368	LEU
1	D	387	ILE
1	D	435	ILE
1	D	453	VAL
1	D	457	ASP

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	HIS
1	B	148	ASN
1	D	69	HIS
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	0.54	0	2,7,9	1.38	0
1	CMH	A	338	1	5,7,8	0.60	0	2,7,9	1.31	0
1	CMH	A	340	1	5,7,8	0.67	0	2,7,9	1.45	0
1	CMH	A	371	1	5,7,8	0.57	0	2,7,9	2.09	1 (50%)
1	CMH	B	264	1	5,7,8	0.83	0	2,7,9	1.79	0
1	CMH	B	338	1	5,7,8	0.59	0	2,7,9	1.42	0
1	CMH	B	340	1	5,7,8	0.51	0	2,7,9	1.22	0
1	CMH	B	371	1	5,7,8	0.48	0	2,7,9	2.07	1 (50%)
1	CMH	C	264	1	5,7,8	0.67	0	2,7,9	1.97	1 (50%)
1	CMH	C	338	1	5,7,8	0.67	0	2,7,9	1.21	0
1	CMH	C	340	1	5,7,8	0.83	0	2,7,9	1.42	0
1	CMH	C	371	1	5,7,8	0.63	0	2,7,9	1.56	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	0.65	0	2,7,9	1.26	0
1	CMH	D	340	1	5,7,8	0.65	0	2,7,9	1.22	0
1	CMH	D	371	1	5,7,8	0.52	0	2,7,9	1.34	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
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	A	371	CMH	O-C-CA	-2.26	119.61	125.49
1	B	371	CMH	CA-CB-SG	2.15	121.82	114.16
1	C	264	CMH	CA-CB-SG	2.34	122.47	114.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	338	CMH	2	0
1	D	340	CMH	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

15 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	B	1471	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	B	1472	-	4,4,4	0.25	0	6,6,6	0.21	0
3	DXC	B	1473	-	28,31,31	1.45	5 (17%)	46,49,49	1.63	10 (21%)
4	5GP	B	1474	-	21,26,26	0.55	0	25,40,40	1.61	5 (20%)
2	SO4	C	1471	-	4,4,4	0.18	0	6,6,6	0.28	0
2	SO4	C	1472	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	C	1473	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	C	1474	-	4,4,4	0.14	0	6,6,6	0.15	0
3	DXC	C	1475	-	28,31,31	1.78	6 (21%)	46,49,49	1.83	15 (32%)
3	DXC	C	1476	-	28,31,31	1.65	5 (17%)	46,49,49	1.63	10 (21%)
3	DXC	C	1477	-	28,31,31	1.61	6 (21%)	46,49,49	1.56	12 (26%)
3	DXC	C	1478	-	28,31,31	1.51	6 (21%)	46,49,49	1.90	13 (28%)
3	DXC	C	1479	-	28,31,31	1.51	6 (21%)	46,49,49	1.93	14 (30%)
3	DXC	C	1480	-	28,31,31	1.82	8 (28%)	46,49,49	1.80	9 (19%)
2	SO4	C	1481	-	4,4,4	0.16	0	6,6,6	0.07	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	B	1471	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1472	-	-	0/0/0/0	0/0/0/0
3	DXC	B	1473	-	-	0/7/71/71	0/4/4/4
4	5GP	B	1474	-	-	0/6/26/26	0/3/3/3
2	SO4	C	1471	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1472	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1473	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1474	-	-	0/0/0/0	0/0/0/0
3	DXC	C	1475	-	-	0/7/71/71	0/4/4/4
3	DXC	C	1476	-	-	0/7/71/71	0/4/4/4
3	DXC	C	1477	-	-	0/7/71/71	0/4/4/4
3	DXC	C	1478	-	-	0/7/71/71	0/4/4/4
3	DXC	C	1479	-	-	0/7/71/71	0/4/4/4
3	DXC	C	1480	-	-	0/7/71/71	0/4/4/4
2	SO4	C	1481	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1475	DXC	C12-C13	-4.62	1.47	1.54
3	C	1480	DXC	C12-C13	-4.23	1.47	1.54
3	C	1477	DXC	C12-C13	-3.95	1.48	1.54
3	C	1480	DXC	C18-C4	-3.72	1.47	1.54
3	C	1476	DXC	C12-C13	-3.53	1.49	1.54
3	C	1475	DXC	C20-C12	-3.41	1.48	1.54
3	C	1476	DXC	C12-C11	-3.29	1.49	1.55
3	C	1476	DXC	O1-C13	-3.25	1.38	1.43
3	C	1477	DXC	C18-C4	-3.19	1.48	1.54
3	C	1478	DXC	C20-C12	-3.16	1.49	1.54
3	B	1473	DXC	C12-C13	-3.10	1.49	1.54
3	B	1473	DXC	C20-C12	-3.01	1.49	1.54
3	C	1476	DXC	C20-C12	-2.99	1.49	1.54
3	C	1475	DXC	C12-C11	-2.98	1.50	1.55
3	C	1478	DXC	C18-C4	-2.90	1.49	1.54
3	C	1480	DXC	C5-C4	-2.86	1.48	1.54
3	C	1480	DXC	C12-C11	-2.86	1.50	1.55
3	C	1478	DXC	C12-C13	-2.85	1.50	1.54
3	C	1479	DXC	C12-C11	-2.82	1.50	1.55
3	C	1480	DXC	O1-C13	-2.82	1.38	1.43
3	C	1479	DXC	C18-C4	-2.70	1.49	1.54
3	C	1475	DXC	C18-C4	-2.68	1.49	1.54
3	C	1475	DXC	O1-C13	-2.67	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1480	DXC	C4-C3	-2.66	1.50	1.55
3	B	1473	DXC	O1-C13	-2.64	1.39	1.43
3	C	1477	DXC	C4-C10	-2.63	1.51	1.56
3	C	1479	DXC	C20-C12	-2.60	1.50	1.54
3	C	1476	DXC	C18-C4	-2.60	1.49	1.54
3	C	1477	DXC	C12-C11	-2.56	1.51	1.55
3	C	1477	DXC	C20-C12	-2.54	1.50	1.54
3	C	1479	DXC	C12-C13	-2.49	1.50	1.54
3	C	1480	DXC	C20-C12	-2.41	1.50	1.54
3	C	1480	DXC	C4-C10	-2.41	1.51	1.56
3	B	1473	DXC	C18-C4	-2.38	1.50	1.54
3	C	1475	DXC	C12-C17	-2.32	1.51	1.55
3	C	1479	DXC	O1-C13	-2.29	1.39	1.43
3	C	1478	DXC	C2-C1	-2.28	1.47	1.51
3	C	1477	DXC	O1-C13	-2.28	1.39	1.43
3	B	1473	DXC	C12-C11	-2.22	1.51	1.55
3	C	1478	DXC	C12-C11	-2.22	1.51	1.55
3	C	1478	DXC	O1-C13	-2.04	1.40	1.43
3	C	1479	DXC	C4-C3	-2.02	1.52	1.55

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1480	DXC	C22-C21-C19	-5.15	108.68	114.75
3	C	1478	DXC	C10-C14-C13	-4.85	108.23	114.36
3	C	1480	DXC	C18-C4-C5	-4.52	100.60	108.20
3	C	1478	DXC	C7-C8-C9	-4.39	104.25	112.10
3	C	1476	DXC	C18-C4-C3	-4.31	102.64	110.25
3	C	1479	DXC	C18-C4-C3	-4.12	102.97	110.25
4	B	1474	5GP	N3-C2-N1	-4.02	121.32	127.44
3	B	1473	DXC	C18-C4-C3	-3.88	103.39	110.25
3	C	1479	DXC	C10-C14-C13	-3.85	109.49	114.36
3	C	1475	DXC	O1-C13-C12	-3.75	105.03	111.11
3	B	1473	DXC	C10-C14-C13	-3.67	109.72	114.36
3	C	1475	DXC	C11-C12-C13	-3.63	104.14	107.39
3	C	1475	DXC	C10-C14-C13	-3.59	109.83	114.36
3	C	1479	DXC	C11-C9-C10	-3.49	104.47	109.06
3	C	1475	DXC	C18-C4-C3	-3.49	104.09	110.25
3	C	1480	DXC	C4-C10-C9	-3.46	108.54	112.40
3	C	1476	DXC	C10-C14-C13	-3.36	110.12	114.36
3	C	1477	DXC	C10-C14-C13	-3.34	110.14	114.36
3	C	1478	DXC	C22-C21-C19	-3.33	110.83	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1476	DXC	C22-C21-C19	-3.27	110.89	114.75
3	C	1475	DXC	C3-C2-C1	-3.27	108.05	112.91
3	C	1478	DXC	C15-C11-C12	-3.27	100.35	103.60
3	C	1479	DXC	C15-C11-C9	-3.23	113.93	119.03
3	C	1476	DXC	C15-C11-C12	-3.14	100.48	103.60
3	C	1479	DXC	C6-C5-C4	-3.09	107.31	112.84
3	C	1477	DXC	C11-C9-C10	-3.04	105.06	109.06
4	B	1474	5GP	C5-C6-N1	-2.96	119.54	123.59
3	C	1478	DXC	C6-C5-C4	-2.92	107.63	112.84
3	C	1479	DXC	C12-C17-C19	-2.90	115.97	119.50
3	B	1473	DXC	C6-C5-C4	-2.90	107.66	112.84
3	C	1477	DXC	C7-C8-C9	-2.89	106.93	112.10
3	B	1473	DXC	C20-C12-C17	-2.86	106.71	111.22
3	C	1476	DXC	C4-C10-C9	-2.82	109.25	112.40
3	C	1475	DXC	C22-C21-C19	-2.76	111.50	114.75
3	C	1478	DXC	C16-C15-C11	-2.75	99.58	105.12
3	C	1478	DXC	C3-C2-C1	-2.75	108.83	112.91
3	C	1479	DXC	C15-C11-C12	-2.73	100.88	103.60
3	C	1475	DXC	C18-C4-C5	-2.72	103.63	108.20
3	C	1476	DXC	C7-C8-C9	-2.71	107.26	112.10
3	C	1480	DXC	C7-C8-C9	-2.70	107.27	112.10
3	C	1477	DXC	C15-C11-C12	-2.69	100.92	103.60
3	C	1480	DXC	C14-C13-C12	-2.66	108.50	111.20
3	C	1478	DXC	C14-C13-C12	-2.61	108.55	111.20
3	C	1477	DXC	C14-C13-C12	-2.60	108.56	111.20
3	C	1480	DXC	C15-C11-C12	-2.57	101.04	103.60
3	C	1478	DXC	C2-C1-C6	-2.56	107.26	110.52
3	C	1476	DXC	C15-C11-C9	-2.53	115.03	119.03
3	C	1475	DXC	C24-C19-C21	-2.52	106.15	110.35
3	C	1475	DXC	C17-C12-C13	-2.46	115.50	117.68
3	C	1475	DXC	C7-C8-C9	-2.44	107.74	112.10
3	C	1479	DXC	C2-C3-C4	-2.36	110.06	112.66
3	C	1477	DXC	C16-C15-C11	-2.34	100.41	105.12
3	C	1477	DXC	C17-C12-C13	-2.32	115.62	117.68
3	C	1478	DXC	C18-C4-C3	-2.30	106.19	110.25
3	C	1478	DXC	C24-C19-C21	-2.30	106.52	110.35
3	C	1479	DXC	C20-C12-C17	-2.28	107.61	111.22
3	B	1473	DXC	C7-C8-C9	-2.23	108.12	112.10
3	C	1475	DXC	C11-C9-C10	-2.15	106.23	109.06
3	B	1473	DXC	C15-C11-C9	-2.11	115.69	119.03
3	C	1475	DXC	C2-C3-C4	-2.09	110.35	112.66
3	C	1479	DXC	C24-C19-C17	-2.09	109.48	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1474	5GP	C4-C5-N7	-2.07	107.58	109.48
3	C	1477	DXC	C6-C5-C4	-2.07	109.14	112.84
4	B	1474	5GP	O2P-P-O5'	-2.03	100.73	106.56
3	C	1479	DXC	C14-C10-C4	-2.02	111.69	113.79
3	C	1476	DXC	C3-C2-C1	-2.02	109.91	112.91
3	C	1477	DXC	C2-C3-C7	-2.01	107.91	111.66
3	C	1475	DXC	C18-C4-C10	2.03	114.22	111.18
3	C	1475	DXC	C17-C12-C11	2.06	102.13	100.05
3	C	1477	DXC	O1-C13-C14	2.11	113.39	109.06
3	B	1473	DXC	C20-C12-C11	2.16	114.62	111.22
3	C	1479	DXC	C5-C4-C3	2.27	111.55	107.81
3	C	1478	DXC	C10-C4-C3	2.35	112.16	108.67
3	C	1478	DXC	C8-C9-C10	2.42	113.35	110.46
3	C	1480	DXC	C10-C4-C3	2.49	112.36	108.67
3	C	1480	DXC	C8-C9-C10	2.55	113.51	110.46
3	C	1477	DXC	C8-C9-C10	2.59	113.56	110.46
3	B	1473	DXC	C18-C4-C10	2.60	115.08	111.18
3	C	1475	DXC	C20-C12-C11	2.61	115.33	111.22
3	B	1473	DXC	C10-C4-C3	2.64	112.58	108.67
3	C	1479	DXC	C18-C4-C10	2.71	115.23	111.18
3	C	1477	DXC	C10-C4-C3	2.84	112.88	108.67
3	B	1473	DXC	C17-C12-C13	3.04	120.38	117.68
3	C	1476	DXC	C8-C9-C10	3.19	114.28	110.46
3	C	1476	DXC	C10-C4-C3	3.33	113.60	108.67
3	C	1480	DXC	C5-C4-C10	3.50	117.09	111.45
4	B	1474	5GP	C6-N1-C2	3.54	120.85	115.94
3	C	1479	DXC	C8-C9-C10	4.60	115.97	110.46

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
2	B	1471	SO4	1	0
3	B	1473	DXC	2	0
4	B	1474	5GP	2	0
2	C	1473	SO4	1	0
3	C	1475	DXC	2	0
3	C	1476	DXC	3	0
3	C	1478	DXC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1479	DXC	3	0
3	C	1480	DXC	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	444/482 (92%)	0.80	79 (17%) 2 1	89, 172, 246, 330	0
1	B	452/482 (93%)	0.86	70 (15%) 3 1	67, 130, 321, 373	0
1	C	467/482 (96%)	0.27	22 (4%) 35 20	65, 105, 204, 279	0
1	D	463/482 (96%)	1.68	144 (31%) 1 0	117, 220, 320, 374	0
All	All	1826/1928 (94%)	0.90	315 (17%) 2 1	65, 163, 299, 374	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	THR	16.9
1	D	442	LYS	12.5
1	D	441	THR	12.5
1	D	453	VAL	11.8
1	B	441	THR	11.3
1	D	406	ILE	10.5
1	D	333	ILE	10.5
1	D	438	THR	10.4
1	D	412	SER	10.2
1	D	415	ALA	9.9
1	B	461	LEU	9.4
1	D	399	ILE	9.4
1	D	401	LYS	9.1
1	B	445	LEU	9.1
1	D	334	SER	8.9
1	D	402	GLY	8.9
1	D	428	GLY	8.8
1	B	450	SER	8.6
1	D	416	ALA	8.6
1	B	330	ASN	8.6
1	A	197	LYS	8.3

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Mol	Chain	Res	Type	RSRZ
1	B	396	LYS	8.2
1	B	432	VAL	8.0
1	D	314	PRO	7.9
1	B	439	PHE	7.8
1	B	460	ILE	7.8
1	B	449	PHE	7.6
1	D	413	LYS	7.6
1	D	426	ILE	7.5
1	D	320	PHE	7.4
1	D	329	LEU	7.2
1	D	439	PHE	7.0
1	B	433	GLY	7.0
1	D	462	ASN	6.9
1	D	400	ASP	6.8
1	B	405	VAL	6.8
1	D	414	VAL	6.8
1	D	411	GLN	6.7
1	D	403	ARG	6.7
1	A	196	ILE	6.7
1	B	397	VAL	6.5
1	D	17	GLY	6.4
1	D	13	HIS	6.4
1	B	424	ILE	6.4
1	D	405	VAL	6.4
1	D	440	GLY	6.3
1	D	444	LEU	6.2
1	B	334	SER	6.1
1	A	230	ARG	6.1
1	D	431	ILE	6.0
1	B	400	ASP	6.0
1	D	467	TRP	6.0
1	D	445	LEU	6.0
1	D	316	LYS	6.0
1	D	330	ASN	5.8
1	D	452	ASN	5.8
1	D	409	LEU	5.8
1	D	318	VAL	5.8
1	B	447	ALA	5.7
1	B	411	GLN	5.6
1	B	418	LYS	5.6
1	D	437	GLY	5.4
1	A	449	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	454	GLU	5.3
1	D	391	VAL	5.3
1	D	449	PHE	5.3
1	B	454	GLU	5.3
1	D	397	VAL	5.2
1	D	356	VAL	5.2
1	D	390	GLU	5.2
1	D	425	SER	5.2
1	D	250	MET	5.2
1	D	429	LYS	5.1
1	B	440	GLY	5.1
1	D	377	GLU	5.1
1	D	417	GLU	5.1
1	D	382	ILE	5.0
1	B	402	GLY	5.0
1	D	392	LEU	5.0
1	B	403	ARG	5.0
1	D	419	LEU	5.0
1	B	409	LEU	5.0
1	D	311	VAL	4.9
1	A	465	ARG	4.9
1	A	198	GLY	4.9
1	D	380	LYS	4.8
1	A	218	LEU	4.8
1	B	457	ASP	4.8
1	D	376	ILE	4.7
1	D	327	ILE	4.7
1	D	407	ASP	4.7
1	B	446	THR	4.7
1	A	389	LYS	4.6
1	D	455	ASN	4.6
1	D	432	VAL	4.6
1	D	424	ILE	4.6
1	A	424	ILE	4.5
1	D	436	LYS	4.5
1	B	453	VAL	4.5
1	D	19	THR	4.4
1	B	428	GLY	4.4
1	A	260	ILE	4.4
1	B	412	SER	4.4
1	D	280	VAL	4.3
1	B	392	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	4.3
1	D	16	HIS	4.3
1	D	461	LEU	4.3
1	B	29	ALA	4.2
1	A	433	GLY	4.2
1	B	399	ILE	4.2
1	D	331	GLU	4.2
1	B	438	THR	4.2
1	D	218	LEU	4.1
1	A	422	GLU	4.1
1	A	259	GLN	4.1
1	A	225	MET	4.1
1	A	273	LEU	4.1
1	D	38	PRO	4.1
1	C	36	LYS	4.0
1	B	429	LYS	4.0
1	A	323	THR	4.0
1	B	329	LEU	3.9
1	C	435	ILE	3.9
1	D	312	ALA	3.9
1	D	332	VAL	3.8
1	A	220	VAL	3.8
1	A	423	GLU	3.8
1	B	442	LYS	3.8
1	D	248	VAL	3.8
1	D	350	ALA	3.8
1	D	459	VAL	3.8
1	A	434	LYS	3.8
1	D	443	GLY	3.7
1	D	249	GLY	3.7
1	A	388	LYS	3.7
1	D	456	ARG	3.6
1	C	410	ALA	3.6
1	A	0	HIS	3.6
1	A	405	VAL	3.6
1	A	322	LYS	3.6
1	D	464	LEU	3.6
1	A	50	GLY	3.6
1	B	414	VAL	3.6
1	D	398	LYS	3.6
1	D	323	THR	3.6
1	B	398	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	416	ALA	3.5
1	B	467	TRP	3.5
1	D	352	VAL	3.5
1	D	385	LEU	3.5
1	B	335	GLY	3.4
1	B	427	GLU	3.4
1	D	328	ILE	3.4
1	D	256	ASP	3.4
1	A	326	ASN	3.4
1	B	293	LEU	3.4
1	D	45	ILE	3.4
1	B	410	ALA	3.4
1	A	448	GLU	3.4
1	B	444	LEU	3.4
1	D	317	LYS	3.3
1	C	35	ASP	3.2
1	C	449	PHE	3.2
1	A	257	ALA	3.2
1	D	321	GLY	3.2
1	B	455	ASN	3.2
1	B	417	GLU	3.2
1	D	384	ASP	3.2
1	B	401	LYS	3.2
1	C	438	THR	3.2
1	D	315	PHE	3.1
1	D	451	GLY	3.1
1	C	409	LEU	3.1
1	D	378	GLU	3.1
1	A	266	LEU	3.1
1	D	322	LYS	3.1
1	D	388	LYS	3.1
1	C	402	GLY	3.1
1	D	339	TYR	3.1
1	D	372	GLY	3.1
1	A	320	PHE	3.1
1	A	255	VAL	3.1
1	B	452	ASN	3.1
1	D	288	ILE	3.1
1	A	460	ILE	3.0
1	B	382	ILE	3.0
1	D	435	ILE	3.0
1	A	426	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	407	ASP	3.0
1	A	271	THR	3.0
1	B	413	LYS	3.0
1	C	442	LYS	3.0
1	D	65	ASP	2.9
1	D	313	VAL	2.9
1	D	187	LYS	2.9
1	D	18	LYS	2.9
1	B	415	ALA	2.9
1	D	28	ILE	2.9
1	D	289	PHE	2.9
1	A	432	VAL	2.9
1	D	179	ILE	2.9
1	D	357	LEU	2.9
1	A	385	LEU	2.8
1	C	413	LYS	2.8
1	D	335	GLY	2.8
1	D	211	ILE	2.8
1	B	443	GLY	2.8
1	D	20	THR	2.8
1	D	383	LYS	2.8
1	A	256	ASP	2.8
1	D	422	GLU	2.8
1	A	252	ILE	2.8
1	A	324	GLU	2.8
1	C	396	LYS	2.8
1	D	430	ASP	2.8
1	A	281	ALA	2.8
1	D	389	LYS	2.8
1	A	464	LEU	2.7
1	B	435	ILE	2.7
1	A	387	ILE	2.7
1	D	220	VAL	2.7
1	B	456	ARG	2.7
1	A	441	THR	2.7
1	C	397	VAL	2.7
1	A	321	GLY	2.7
1	C	406	ILE	2.7
1	A	203	VAL	2.7
1	C	419	LEU	2.7
1	A	435	ILE	2.7
1	A	379	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	292	ASN	2.6
1	B	434	LYS	2.6
1	D	326	ASN	2.6
1	A	276	VAL	2.6
1	A	330	ASN	2.6
1	B	406	ILE	2.6
1	A	376	ILE	2.5
1	A	72	LEU	2.5
1	A	392	LEU	2.5
1	B	331	GLU	2.5
1	D	458	LYS	2.5
1	D	295	PRO	2.5
1	B	393	ARG	2.5
1	D	268	SER	2.5
1	B	468	GLY	2.5
1	A	65	ASP	2.5
1	A	305	MET	2.5
1	A	390	GLU	2.5
1	B	389	LYS	2.5
1	D	374	GLY	2.5
1	B	311	VAL	2.5
1	B	387	ILE	2.5
1	D	285	ILE	2.5
1	D	286	SER	2.4
1	A	341	ALA	2.4
1	A	436	LYS	2.4
1	D	219	LYS	2.4
1	A	466	ARG	2.4
1	A	386	ASN	2.4
1	C	424	ILE	2.4
1	A	194	PHE	2.4
1	A	396	LYS	2.4
1	A	406	ILE	2.4
1	D	325	GLU	2.4
1	A	279	ILE	2.4
1	D	66	ALA	2.4
1	C	411	GLN	2.4
1	A	204	THR	2.3
1	D	393	ARG	2.3
1	A	242	ALA	2.3
1	B	292	ASN	2.3
1	A	346	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	423	GLU	2.3
1	D	457	ASP	2.3
1	C	414	VAL	2.3
1	D	341	ALA	2.3
1	D	319	THR	2.3
1	A	291	TYR	2.2
1	A	431	ILE	2.2
1	D	303	VAL	2.2
1	C	417	GLU	2.2
1	C	467	TRP	2.2
1	A	398	LYS	2.2
1	B	458	LYS	2.2
1	D	181	ASN	2.2
1	A	51	PHE	2.2
1	D	228	LYS	2.2
1	A	253	GLN	2.2
1	B	315	PHE	2.2
1	A	462	ASN	2.2
1	D	279	ILE	2.1
1	D	290	LYS	2.1
1	C	444	LEU	2.1
1	A	404	THR	2.1
1	D	296	LYS	2.1
1	D	251	ALA	2.1
1	D	169	ILE	2.1
1	C	42	LYS	2.1
1	D	465	ARG	2.1
1	A	459	VAL	2.1
1	D	418	LYS	2.1
1	D	69	HIS	2.1
1	C	439	PHE	2.1
1	A	199	ALA	2.1
1	D	78	SER	2.1
1	D	173	LEU	2.1
1	D	460	ILE	2.0
1	A	382	ILE	2.0
1	A	317	LYS	2.0
1	D	404	THR	2.0
1	A	250	MET	2.0
1	D	241	GLU	2.0
1	A	319	THR	2.0
1	A	347	LYS	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	338	8/9	0.75	0.17	-	187,264,268,302	2
1	CMH	B	338	8/9	0.95	0.15	-	157,190,227,235	2
1	CMH	D	371	8/9	0.96	0.21	-	129,151,184,191	2
1	CMH	B	264	8/9	1.00	0.23	-	57,72,95,100	2
1	CMH	A	264	8/9	0.98	0.17	-	166,181,195,201	2
1	CMH	B	371	8/9	0.94	0.13	-	141,161,218,263	2
1	CMH	C	371	8/9	1.00	0.19	-	55,102,148,154	2
1	CMH	A	371	8/9	0.91	0.34	-	154,165,195,202	2
1	CMH	C	338	8/9	0.97	0.19	-	72,94,152,200	2
1	CMH	C	264	8/9	1.00	0.17	-	61,95,114,120	0
1	CMH	D	340	8/9	0.96	0.24	-	155,269,276,276	2
1	CMH	B	340	8/9	0.98	0.17	-	141,161,259,276	2
1	CMH	C	340	8/9	0.98	0.16	-	58,87,108,131	2
1	CMH	A	338	8/9	0.94	0.21	-	149,179,204,211	2
1	CMH	A	340	8/9	0.98	0.22	-	150,189,198,212	2
1	CMH	D	264	8/9	0.98	0.24	-	164,180,206,220	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
2	SO4	B	1472	5/5	0.91	0.42	5.48	94,222,224,320	0
3	DXC	C	1476	28/28	0.89	0.34	1.16	139,146,204,235	0
3	DXC	C	1479	28/28	0.93	0.34	1.12	72,89,173,216	28

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DXC	C	1477	28/28	0.95	0.30	0.99	67,90,157,199	0
2	SO4	C	1471	5/5	0.96	0.24	0.76	93,127,147,181	0
3	DXC	C	1478	28/28	0.96	0.31	0.73	73,105,138,168	0
4	5GP	B	1474	24/24	0.88	0.41	0.72	204,243,284,292	0
3	DXC	B	1473	28/28	0.98	0.26	0.25	62,82,119,128	0
3	DXC	C	1475	28/28	0.97	0.26	0.15	64,79,119,144	0
3	DXC	C	1480	28/28	0.98	0.23	-0.33	64,76,98,107	0
2	SO4	C	1473	5/5	0.88	0.11	-	138,173,210,226	5
2	SO4	C	1472	5/5	0.96	0.17	-	112,131,153,180	0
2	SO4	C	1481	5/5	0.66	0.85	-	157,190,196,199	5
2	SO4	B	1471	5/5	0.73	0.42	-	172,203,237,246	0
2	SO4	C	1474	5/5	0.56	0.62	-	156,216,245,297	5

6.5 Other polymers (i)

There are no such residues in this entry.