



Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2016 – 06:08 PM EDT

PDB ID : 5CNT
Title : Crystal structure of the dATP inhibited E. coli class Ia ribonucleotide reductase complex bound to UDP and dATP at 3.25 Angstroms resolution
Authors : Chen, P.Y.-T.; Zimanyi, C.M.; Funk, M.A.; Drennan, C.L.
Deposited on : 2015-07-18
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

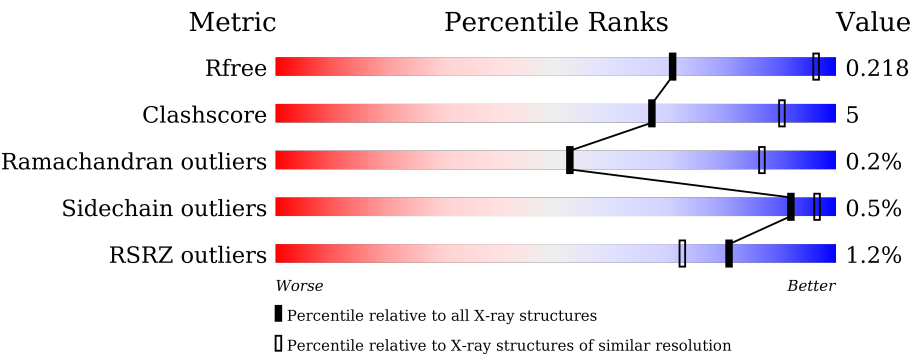
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

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 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	<div><div>%</div><div><div></div><div>83%</div><div>13%</div><div>..</div></div></div>
1	B	761	<div><div></div><div><div>84%</div><div>13%</div><div>.</div></div></div>
1	C	761	<div><div>4%</div><div><div></div><div>83%</div><div>13%</div><div>.</div></div></div>
1	D	761	<div><div>%</div><div><div></div><div>84%</div><div>12%</div><div>.</div></div></div>
2	E	375	<div><div>2%</div><div><div></div><div>82%</div><div>11%</div><div>7%</div></div></div>
2	F	375	<div><div></div><div><div></div><div>83%</div><div>12%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	375	<div><div></div><div>82%</div><div>14%</div><div>5%</div></div>
2	H	375	<div><div>2%</div><div></div><div>82%</div><div>13%</div><div>5%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35437 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.

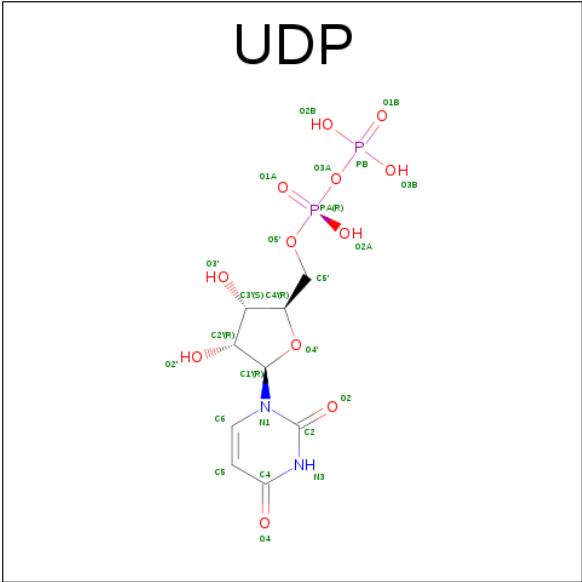
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5845	3712	1004	1105	24			
1	B	734	Total	C	N	O	S	0	0	0
			5845	3712	1004	1105	24			
1	C	734	Total	C	N	O	S	0	0	0
			5836	3705	1003	1104	24			
1	D	733	Total	C	N	O	S	0	0	0
			5835	3706	1003	1102	24			

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

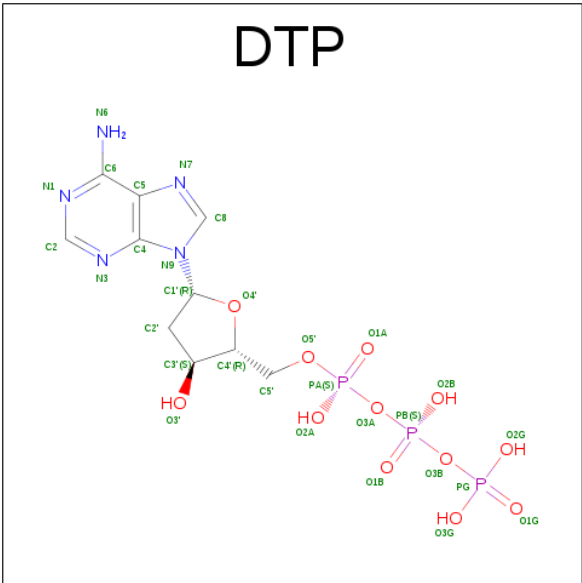
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	350	Total	C	N	O	S	0	0	0
			2840	1814	470	543	13			
2	F	357	Total	C	N	O	S	0	0	0
			2915	1860	482	560	13			
2	G	357	Total	C	N	O	S	0	0	0
			2895	1852	477	553	13			
2	H	355	Total	C	N	O	S	0	0	0
			2887	1845	478	551	13			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).

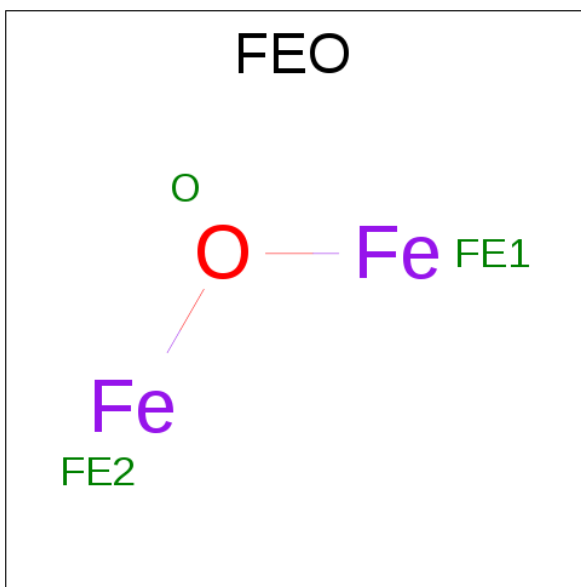


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		
5	A	2	Total	Mg	0	0
			2	2		
5	D	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe₂O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	Fe	O	0	0
			3	2	1		
6	F	1	Total	Fe	O	0	0
			3	2	1		
6	G	1	Total	Fe	O	0	0
			3	2	1		
6	H	1	Total	Fe	O	0	0
			3	2	1		

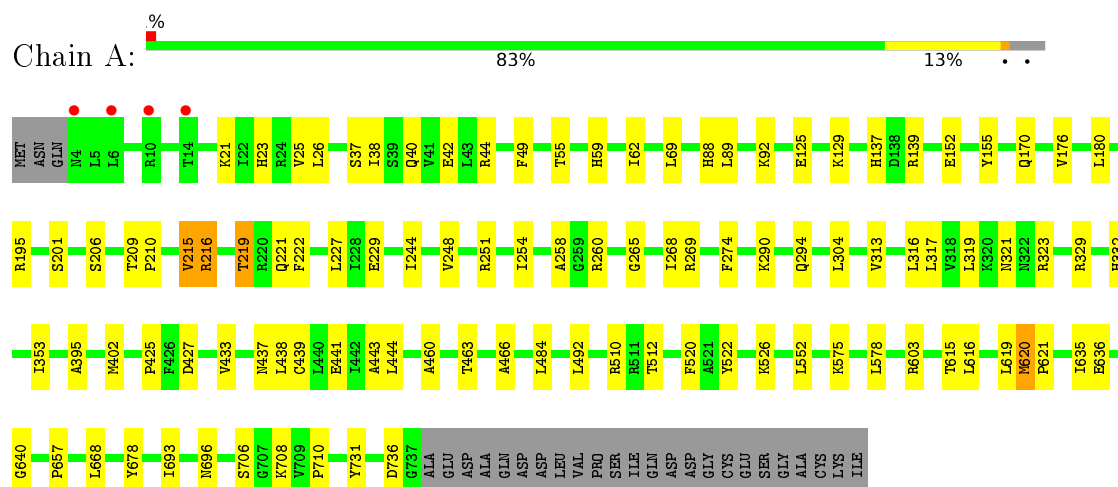
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total	O	0	0
			14	14		
7	B	12	Total	O	0	0
			12	12		
7	C	4	Total	O	0	0
			4	4		
7	D	6	Total	O	0	0
			6	6		
7	E	3	Total	O	0	0
			3	3		
7	F	6	Total	O	0	0
			6	6		
7	G	9	Total	O	0	0
			9	9		
7	H	5	Total	O	0	0
			5	5		

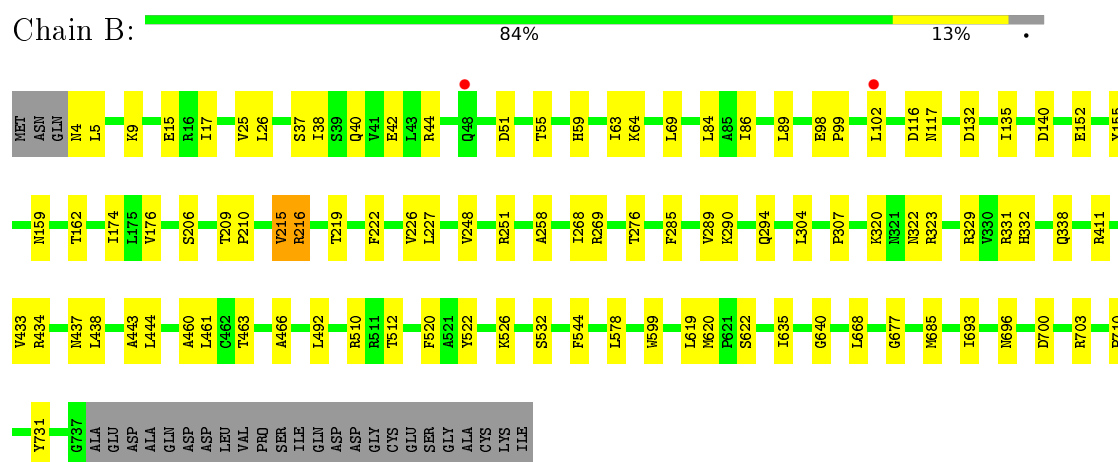
3 Residue-property plots

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.

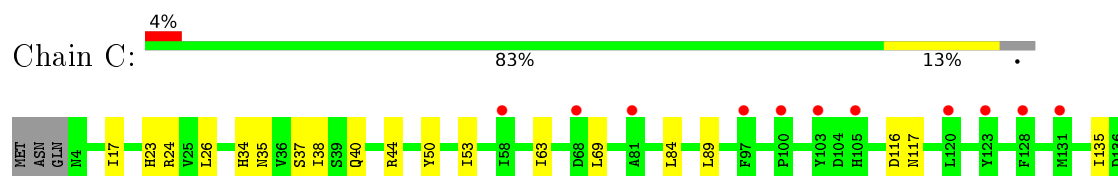
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



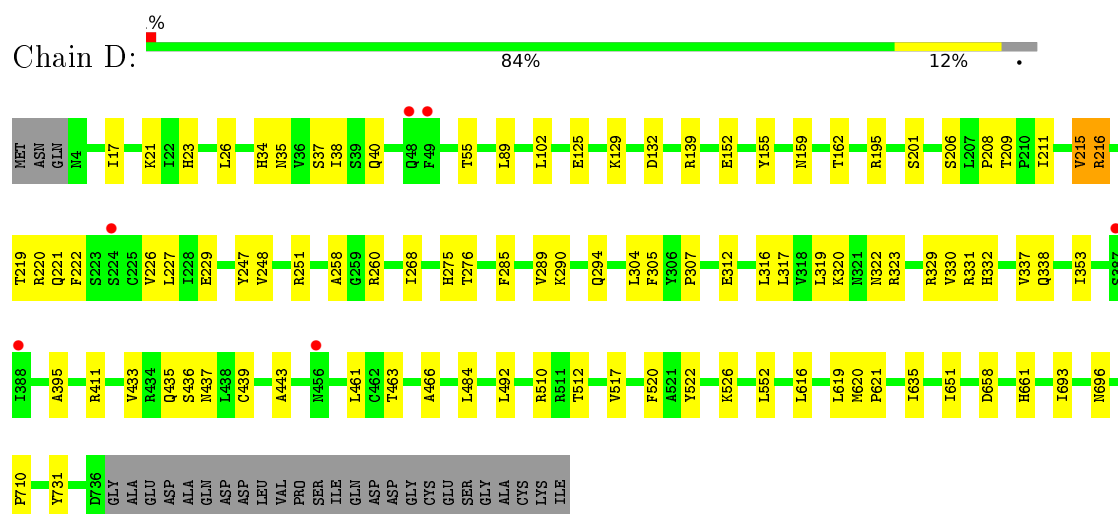
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



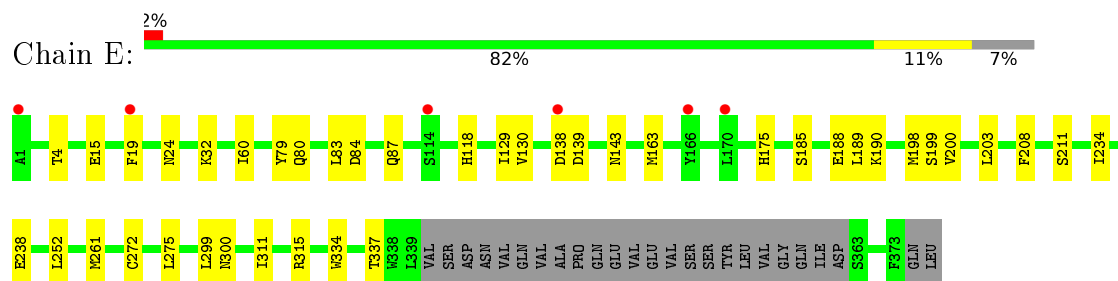
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



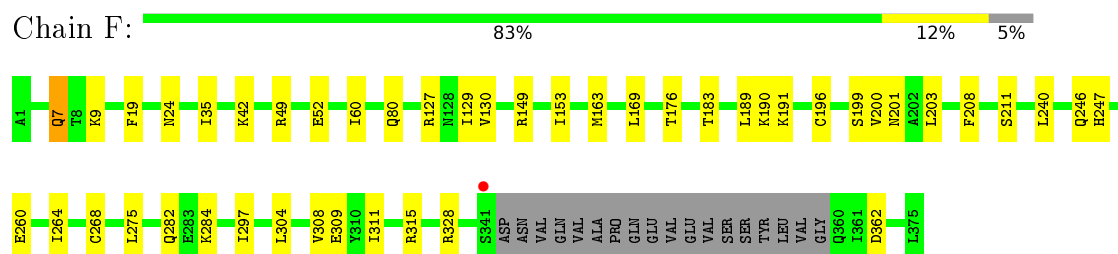
- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



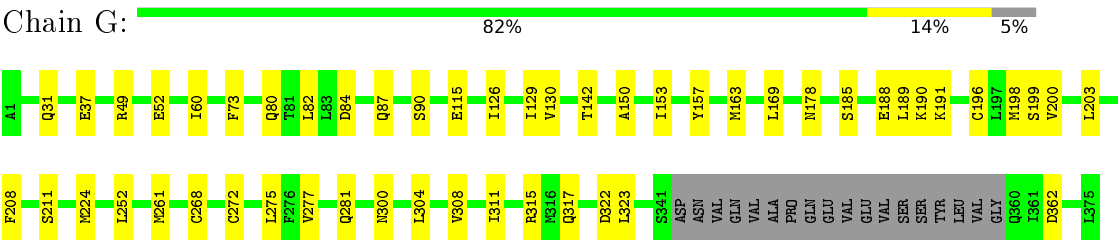
- Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



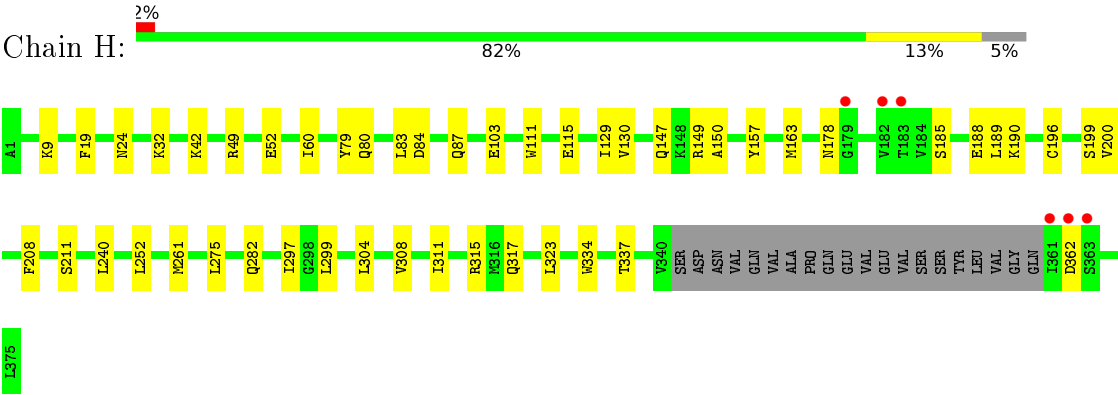
- Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



- Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



● Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	274.62Å 157.34Å 165.20Å 90.00° 119.30° 90.00°	Depositor
Resolution (Å)	49.95 – 3.25 49.95 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.95-3.25) 97.8 (49.95-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.192 , 0.221 0.187 , 0.218	Depositor DCC
R_{free} test set	4754 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35437	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FEO, MG, DTP, UDP

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	0.26	0/5973	0.43	0/8090
1	B	0.26	0/5973	0.43	0/8090
1	C	0.25	0/5964	0.42	0/8078
1	D	0.25	0/5963	0.42	0/8077
2	E	0.24	0/2903	0.39	0/3940
2	F	0.27	0/2979	0.42	0/4041
2	G	0.27	0/2959	0.41	0/4015
2	H	0.25	0/2951	0.40	0/4004
All	All	0.26	0/35665	0.42	0/48335

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5845	0	5770	69	0
1	B	5845	0	5770	57	0
1	C	5836	0	5748	55	0
1	D	5835	0	5756	55	0
2	E	2840	0	2749	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2915	0	2832	29	0
2	G	2895	0	2804	29	0
2	H	2887	0	2800	29	0
3	A	25	0	11	2	0
3	B	25	0	11	3	0
3	C	25	0	11	3	0
3	D	25	0	11	2	0
4	A	90	0	36	2	0
4	B	90	0	36	4	0
4	C	90	0	36	1	0
4	D	90	0	36	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	E	3	0	0	0	0
6	F	3	0	0	0	0
6	G	3	0	0	1	0
6	H	3	0	0	0	0
7	A	14	0	0	1	0
7	B	12	0	0	1	0
7	C	4	0	0	0	0
7	D	6	0	0	1	0
7	E	3	0	0	1	0
7	F	6	0	0	0	0
7	G	9	0	0	0	0
7	H	5	0	0	0	0
All	All	35437	0	34417	333	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 5.

All (333) 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:322:ASN:HA	1:D:331:ARG:HE	1.39	0.87
1:C:229:GLU:OE2	1:C:260:ARG:NH1	2.17	0.77
1:D:229:GLU:OE2	1:D:260:ARG:NH1	2.19	0.74
1:B:26:LEU:HB3	1:B:38:ILE:HD12	1.72	0.70
1:B:222:PHE:CD2	1:B:492:LEU:HD11	2.27	0.69
1:C:498:TYR:HB2	1:C:504:LYS:HE3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ASN:ND2	3:C:801:UDP:O3'	2.28	0.67
1:A:49:PHE:HE2	2:F:297:ILE:HD11	1.58	0.67
1:B:322:ASN:HA	1:B:331:ARG:HE	1.60	0.67
1:A:321:ASN:HD21	1:A:323:ARG:CZ	2.06	0.67
1:A:221:GLN:NE2	7:A:901:HOH:O	2.27	0.66
1:A:222:PHE:CD2	1:A:492:LEU:HD11	2.31	0.66
1:D:125:GLU:HG2	1:D:129:LYS:HE2	1.78	0.66
1:C:206:SER:HB3	1:C:466:ALA:HB3	1.77	0.66
1:A:229:GLU:OE2	1:A:260:ARG:NH1	2.29	0.65
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.78	0.65
2:F:199:SER:HA	2:F:275:LEU:HD21	1.79	0.64
2:G:199:SER:HA	2:G:275:LEU:HD21	1.80	0.63
1:C:322:ASN:HA	1:C:331:ARG:HE	1.63	0.63
2:H:80:GLN:NE2	2:H:211:SER:OG	2.31	0.62
1:D:258:ALA:HB3	1:D:304:LEU:HD21	1.82	0.62
1:B:251:ARG:HA	1:B:294:GLN:HB3	1.81	0.61
1:C:222:PHE:CD2	1:C:492:LEU:HD11	2.35	0.61
2:G:80:GLN:NE2	2:G:211:SER:OG	2.31	0.61
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.83	0.60
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.84	0.60
1:A:139:ARG:NH1	1:A:201:SER:OG	2.35	0.59
1:C:26:LEU:HB3	1:C:38:ILE:HD12	1.83	0.59
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.83	0.59
2:E:238:GLU:OE1	7:E:601:HOH:O	2.17	0.58
1:C:251:ARG:HA	1:C:294:GLN:HB3	1.84	0.58
2:E:175:HIS:HB3	2:H:178:ASN:HD21	1.68	0.58
1:C:532:SER:HA	1:C:677:GLY:HA3	1.86	0.58
1:A:89:LEU:HD11	1:A:152:GLU:HB3	1.85	0.58
1:B:89:LEU:HD11	1:B:152:GLU:HB3	1.86	0.58
2:E:80:GLN:NE2	2:E:211:SER:OG	2.35	0.57
1:A:59:HIS:HD2	1:A:88:HIS:HB2	1.67	0.57
1:C:268:ILE:HG22	1:C:269:ARG:HD3	1.86	0.57
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.87	0.57
2:F:169:LEU:HD12	2:G:169:LEU:HD12	1.87	0.57
1:A:251:ARG:HA	1:A:294:GLN:HB3	1.87	0.56
1:C:455:GLU:O	1:C:505:ARG:NE	2.38	0.56
1:D:552:LEU:HD23	1:D:616:LEU:HD12	1.89	0.55
1:A:195:ARG:HD2	1:A:484:LEU:HD11	1.89	0.55
1:D:222:PHE:CD2	1:D:492:LEU:HD11	2.42	0.55
1:A:155:TYR:HE1	1:A:209:THR:HG23	1.72	0.55
2:F:80:GLN:NE2	2:F:211:SER:OG	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:PRO:HA	2:G:362:ASP:HB3	1.88	0.55
1:B:640:GLY:HA2	1:B:668:LEU:HD13	1.89	0.55
1:B:338:GLN:NE2	1:B:434:ARG:O	2.38	0.55
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.89	0.55
2:H:252:LEU:HB3	2:H:261:MET:HG2	1.90	0.54
1:A:176:VAL:HG22	1:A:215:VAL:HB	1.89	0.54
1:B:710:PRO:HA	2:H:362:ASP:HB3	1.89	0.54
1:B:55:THR:HG21	4:B:802:DTP:O2B	2.07	0.54
1:A:321:ASN:O	1:A:329:ARG:NE	2.31	0.54
1:D:226:VAL:HG22	1:D:461:LEU:HD22	1.89	0.54
2:G:191:LYS:HG3	2:G:268:CYS:SG	2.47	0.53
1:B:206:SER:HB3	1:B:466:ALA:HB3	1.88	0.53
1:C:576:GLY:HA3	1:C:607:LYS:HE3	1.90	0.53
2:H:19:PHE:CE2	2:H:190:LYS:HG2	2.44	0.53
1:B:463:THR:HG21	1:B:492:LEU:HD23	1.89	0.53
1:C:341:LYS:HG2	1:C:418:ASP:OD2	2.09	0.53
1:A:463:THR:HG21	1:A:492:LEU:HD23	1.90	0.53
1:D:696:ASN:OD1	1:D:731:TYR:HB2	2.09	0.53
2:G:252:LEU:HB3	2:G:261:MET:HG2	1.90	0.53
1:B:42:GLU:HB3	2:H:297:ILE:HG23	1.90	0.53
2:G:153:ILE:HD13	2:G:203:LEU:HD13	1.91	0.52
1:A:427:ASP:OD2	1:A:575:LYS:NZ	2.42	0.52
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.45	0.52
2:E:252:LEU:HD22	2:E:261:MET:HG2	1.90	0.52
1:D:510:ARG:HB2	1:D:512:THR:HG23	1.90	0.52
1:D:323:ARG:O	1:D:329:ARG:NH2	2.43	0.51
1:A:210:PRO:HB2	1:A:222:PHE:HA	1.93	0.51
1:C:23:HIS:CD2	2:E:300:ASN:HD22	2.28	0.51
2:H:79:TYR:CZ	2:H:83:LEU:HD11	2.45	0.51
1:C:219:THR:HG23	1:C:251:ARG:HH22	1.75	0.51
2:F:60:ILE:HD12	2:F:60:ILE:H	1.76	0.51
1:A:317:LEU:HD11	1:A:402:MET:HG3	1.93	0.51
2:G:317:GLN:HB2	2:G:323:LEU:HD21	1.91	0.51
1:B:510:ARG:HB2	1:B:512:THR:HG23	1.93	0.51
1:B:86:ILE:HG21	1:B:140:ASP:HB3	1.93	0.51
2:G:129:ILE:HG13	2:G:130:VAL:HG13	1.93	0.51
1:A:42:GLU:HB3	2:F:297:ILE:HG23	1.92	0.51
2:E:129:ILE:HG13	2:E:130:VAL:HG13	1.93	0.51
2:E:199:SER:HA	2:E:275:LEU:HD21	1.93	0.51
1:A:26:LEU:HD21	1:A:62:ILE:HD12	1.92	0.51
1:C:510:ARG:HB2	1:C:512:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:PHE:CE2	2:F:190:LYS:HG2	2.45	0.50
2:G:277:VAL:O	2:G:281:GLN:HG2	2.12	0.50
1:D:208:PRO:HD2	1:D:211:ILE:HD12	1.94	0.50
1:D:619:LEU:HB2	1:D:693:ILE:HG23	1.92	0.50
2:H:311:ILE:O	2:H:315:ARG:HG2	2.11	0.50
1:B:290:LYS:HE3	1:B:332:HIS:HB3	1.92	0.50
2:E:4:THR:HG21	2:H:157:TYR:HB3	1.94	0.50
2:F:311:ILE:O	2:F:315:ARG:HG2	2.11	0.50
1:A:26:LEU:HB3	1:A:38:ILE:HD12	1.94	0.50
1:A:265:GLY:HA2	1:A:274:PHE:CZ	2.47	0.49
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.93	0.49
1:B:248:VAL:O	1:B:294:GLN:HA	2.12	0.49
1:B:532:SER:HA	1:B:677:GLY:HA3	1.92	0.49
1:C:44:ARG:HG3	1:C:69:LEU:HD21	1.93	0.49
1:B:320:LYS:HE2	1:B:411:ARG:HB2	1.94	0.49
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.47	0.49
1:C:438:LEU:HD23	3:C:801:UDP:H2'	1.94	0.49
1:D:206:SER:HB3	1:D:466:ALA:HB3	1.94	0.49
1:D:21:LYS:NZ	4:D:804:DTP:O3G	2.45	0.49
1:A:125:GLU:HG2	1:A:129:LYS:HE2	1.94	0.49
1:B:437:ASN:ND2	3:B:801:UDP:O3'	2.46	0.49
2:E:185:SER:HB3	2:E:188:GLU:HB2	1.95	0.49
2:H:190:LYS:HD3	2:H:261:MET:HE1	1.94	0.49
1:A:44:ARG:HG3	1:A:69:LEU:HD21	1.95	0.49
1:B:37:SER:HB3	1:B:40:GLN:HB2	1.94	0.49
2:H:24:ASN:N	2:H:24:ASN:OD1	2.43	0.49
1:A:620:MET:SD	1:A:620:MET:N	2.83	0.49
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.95	0.49
1:D:251:ARG:HA	1:D:294:GLN:HB3	1.93	0.48
2:F:309:GLU:OE1	2:F:328:ARG:NH2	2.42	0.48
1:D:353:ILE:HG13	1:D:395:ALA:HB2	1.95	0.48
1:D:276:THR:OG1	4:D:805:DTP:H2	2.14	0.48
1:A:317:LEU:HD12	1:A:402:MET:HA	1.95	0.48
1:B:5:LEU:HD22	1:B:51:ASP:HB2	1.96	0.48
1:C:578:LEU:HD13	1:C:599:TRP:HE3	1.79	0.48
2:F:191:LYS:HG3	2:F:268:CYS:SG	2.53	0.48
1:A:248:VAL:O	1:A:294:GLN:HA	2.13	0.48
2:F:7:GLN:HE21	2:F:7:GLN:HA	1.79	0.48
2:H:129:ILE:HG13	2:H:130:VAL:HG13	1.95	0.48
1:A:313:VAL:O	1:A:317:LEU:HD23	2.13	0.48
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HG3	1:B:69:LEU:HD21	1.95	0.48
1:A:710:PRO:HA	2:F:362:ASP:HB3	1.95	0.48
1:A:438:LEU:HD23	3:A:801:UDP:H2'	1.95	0.48
1:C:34:HIS:CD2	1:C:35:ASN:HB2	2.47	0.48
1:A:59:HIS:CD2	1:A:88:HIS:HB2	2.48	0.48
1:D:55:THR:HG21	4:D:802:DTP:O1B	2.14	0.48
2:H:32:LYS:N	2:H:103:GLU:OE2	2.46	0.48
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.95	0.48
1:C:621:PRO:HB2	1:C:623:GLU:HG2	1.96	0.48
1:D:89:LEU:HD11	1:D:152:GLU:HB3	1.95	0.48
2:F:191:LYS:HE3	2:F:268:CYS:SG	2.53	0.48
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.94	0.47
1:B:63:ILE:HG12	1:B:84:LEU:HB3	1.95	0.47
1:D:290:LYS:HE3	1:D:332:HIS:HB3	1.96	0.47
1:A:221:GLN:O	1:A:251:ARG:NH1	2.46	0.47
1:A:244:ILE:HG12	1:A:254:ILE:HG21	1.96	0.47
1:A:578:LEU:HD11	1:A:603:ARG:HB2	1.96	0.47
1:D:463:THR:HG21	1:D:492:LEU:HD23	1.96	0.47
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.97	0.47
1:A:25:VAL:HG22	4:A:804:DTP:O3'	2.15	0.47
1:C:168:SER:OG	1:C:169:ALA:N	2.47	0.47
1:D:307:PRO:HA	1:D:338:GLN:HB2	1.96	0.47
1:D:320:LYS:HE2	1:D:411:ARG:HB2	1.96	0.47
1:D:26:LEU:HB3	1:D:38:ILE:HD12	1.96	0.47
2:F:9:LYS:HD2	2:G:142:THR:CG2	2.44	0.47
1:B:102:LEU:N	1:B:132:ASP:OD2	2.39	0.47
2:G:115:GLU:CD	6:G:501:FEO:O	2.53	0.47
2:H:163:MET:HB3	2:H:189:LEU:HD13	1.96	0.47
1:D:34:HIS:CD2	1:D:35:ASN:HB2	2.50	0.47
2:F:153:ILE:HD13	2:F:203:LEU:HD13	1.96	0.46
1:B:176:VAL:HG22	1:B:215:VAL:HB	1.97	0.46
1:B:9:LYS:HD3	1:B:15:GLU:HG2	1.96	0.46
1:D:37:SER:HB3	1:D:40:GLN:HB2	1.97	0.46
2:H:185:SER:HB3	2:H:188:GLU:HB2	1.97	0.46
1:A:23:HIS:ND1	1:A:42:GLU:OE2	2.49	0.46
1:B:307:PRO:HA	1:B:338:GLN:HB2	1.97	0.46
1:C:226:VAL:HG22	1:C:461:LEU:HD22	1.98	0.46
2:G:84:ASP:HA	2:G:87:GLN:HB2	1.97	0.46
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.96	0.46
1:D:268:ILE:HD11	1:D:275:HIS:HA	1.98	0.46
2:F:196:CYS:O	2:F:200:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.98	0.46
1:B:438:LEU:HD23	3:B:801:UDP:H2'	1.98	0.46
1:C:290:LYS:HE3	1:C:332:HIS:HB3	1.97	0.46
1:C:353:ILE:HG13	1:C:395:ALA:HB2	1.98	0.46
2:G:304:LEU:O	2:G:308:VAL:HG23	2.16	0.46
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.51	0.46
1:C:619:LEU:HB2	1:C:693:ILE:HG23	1.96	0.46
1:D:522:TYR:CZ	1:D:526:LYS:HD3	2.51	0.45
2:F:176:THR:HG23	2:G:178:ASN:HA	1.98	0.45
1:D:139:ARG:NH1	1:D:201:SER:OG	2.49	0.45
1:D:155:TYR:HE1	1:D:209:THR:HG23	1.81	0.45
1:A:219:THR:HG23	1:A:251:ARG:HH22	1.80	0.45
2:G:49:ARG:O	2:G:52:GLU:HG2	2.16	0.45
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.98	0.45
1:C:24:ARG:NH1	4:C:804:DTP:H1'	2.32	0.45
1:D:305:PHE:CZ	1:D:436:SER:HB3	2.51	0.45
1:D:195:ARG:HB3	1:D:484:LEU:HD21	1.99	0.45
2:E:311:ILE:O	2:E:315:ARG:HG2	2.17	0.45
2:G:163:MET:HB3	2:G:189:LEU:HD13	1.98	0.45
1:A:268:ILE:HG22	1:A:269:ARG:HD3	1.98	0.45
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.98	0.45
1:D:219:THR:HG23	1:D:251:ARG:HH22	1.82	0.45
1:D:621:PRO:HG2	3:D:801:UDP:O2A	2.17	0.45
2:E:200:VAL:HA	2:E:203:LEU:HG	1.99	0.45
2:H:84:ASP:HA	2:H:87:GLN:HB2	1.99	0.45
1:A:290:LYS:HE3	1:A:332:HIS:HB3	1.97	0.45
2:E:139:ASP:O	2:E:143:ASN:HB2	2.17	0.45
2:E:24:ASN:OD1	2:E:24:ASN:N	2.43	0.45
2:F:284:LYS:HG3	2:F:308:VAL:HG11	1.99	0.44
1:C:135:ILE:HD11	1:C:174:ILE:HG21	2.00	0.44
1:D:220:ARG:HA	1:D:222:PHE:CZ	2.53	0.44
1:D:651:ILE:H	1:D:651:ILE:HG13	1.65	0.44
1:B:210:PRO:HB2	1:B:222:PHE:HA	1.99	0.44
1:C:450:ASN:ND2	1:C:454:ASP:OD1	2.49	0.44
2:E:138:ASP:HB3	2:H:9:LYS:HE3	1.99	0.44
1:B:59:HIS:HB2	4:B:802:DTP:H4'	1.99	0.44
2:G:82:LEU:HD11	2:G:150:ALA:HB2	1.99	0.44
1:A:206:SER:HB3	1:A:466:ALA:HB3	1.99	0.44
1:A:222:PHE:HB2	1:A:492:LEU:HD21	1.99	0.44
1:D:517:VAL:HG22	1:D:619:LEU:HD22	1.99	0.44
2:E:15:GLU:O	2:E:32:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:HIS:CD2	2:E:234:ILE:HG12	2.52	0.44
2:E:84:ASP:HA	2:E:87:GLN:HB2	1.98	0.44
1:C:622:SER:N	3:C:801:UDP:O2A	2.51	0.44
1:A:21:LYS:O	1:A:25:VAL:HG23	2.18	0.44
1:C:418:ASP:OD1	1:C:419:HIS:N	2.51	0.44
1:D:102:LEU:N	1:D:132:ASP:OD2	2.45	0.44
1:D:227:LEU:HD23	1:D:435:GLN:HG3	2.00	0.44
2:F:149:ARG:HD3	2:F:282:GLN:HB3	2.00	0.44
1:D:215:VAL:O	1:D:216:ARG:HB3	2.18	0.43
1:A:55:THR:HG21	4:A:802:DTP:O1B	2.18	0.43
2:H:111:TRP:O	2:H:115:GLU:HG2	2.18	0.43
2:H:196:CYS:O	2:H:200:VAL:HG23	2.17	0.43
2:H:149:ARG:HG2	2:H:282:GLN:OE1	2.18	0.43
1:D:520:PHE:HB3	1:D:635:ILE:HA	2.01	0.43
2:F:129:ILE:HG13	2:F:130:VAL:HG13	2.00	0.43
1:B:276:THR:OG1	4:B:805:DTP:H2	2.18	0.43
1:B:619:LEU:HB2	1:B:693:ILE:HG23	2.00	0.43
1:C:313:VAL:O	1:C:317:LEU:HD23	2.18	0.43
2:F:260:GLU:HG2	2:F:264:ILE:HD11	2.00	0.43
1:A:88:HIS:NE2	1:A:92:LYS:HE3	2.33	0.43
1:B:159:ASN:HB3	1:B:162:THR:HB	2.01	0.43
1:B:268:ILE:HG22	1:B:269:ARG:HD3	1.99	0.43
2:G:198:MET:HG3	2:G:272:CYS:SG	2.59	0.43
1:D:247:TYR:OH	1:D:461:LEU:HD11	2.19	0.43
2:F:304:LEU:O	2:F:308:VAL:HG23	2.19	0.43
2:G:311:ILE:O	2:G:315:ARG:HG2	2.19	0.43
1:A:696:ASN:OD1	1:A:731:TYR:HB2	2.19	0.43
2:E:79:TYR:CZ	2:E:83:LEU:HD11	2.54	0.43
2:G:190:LYS:HD3	2:G:261:MET:HE1	2.01	0.43
2:H:199:SER:HA	2:H:275:LEU:HD21	2.00	0.43
1:C:208:PRO:HD2	1:C:211:ILE:HD12	2.01	0.42
2:F:49:ARG:O	2:F:52:GLU:HG2	2.19	0.42
2:H:304:LEU:O	2:H:308:VAL:HG23	2.19	0.42
1:C:208:PRO:HB2	1:C:210:PRO:HD2	2.01	0.42
1:D:159:ASN:HB3	1:D:162:THR:HB	2.01	0.42
2:H:60:ILE:HD12	2:H:60:ILE:H	1.84	0.42
1:A:510:ARG:HB2	1:A:512:THR:HG23	2.01	0.42
2:G:60:ILE:HD12	2:G:60:ILE:H	1.84	0.42
2:G:73:PHE:CZ	2:G:224:MET:HE2	2.55	0.42
1:A:215:VAL:O	1:A:216:ARG:HB3	2.19	0.42
1:A:222:PHE:HD2	1:A:492:LEU:HD11	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:HG21	4:B:802:DTP:H3'	2.01	0.42
2:E:163:MET:HB3	2:E:189:LEU:HD13	2.00	0.42
2:E:60:ILE:H	2:E:60:ILE:HD12	1.83	0.42
2:H:317:GLN:HB2	2:H:323:LEU:HD21	2.02	0.42
1:D:221:GLN:O	1:D:251:ARG:NH1	2.51	0.42
1:D:437:ASN:HB2	7:D:901:HOH:O	2.20	0.42
2:G:185:SER:HB3	2:G:188:GLU:HB2	2.01	0.42
2:H:334:TRP:O	2:H:337:THR:HG22	2.19	0.42
1:B:215:VAL:O	1:B:216:ARG:HB3	2.20	0.42
1:C:176:VAL:O	1:C:180:LEU:HG	2.18	0.42
1:B:222:PHE:HB2	1:B:492:LEU:HD21	2.02	0.42
1:B:437:ASN:HB2	7:B:903:HOH:O	2.19	0.42
1:A:353:ILE:HG13	1:A:395:ALA:HB2	2.02	0.42
1:A:522:TYR:HB2	1:A:657:PRO:HG2	2.02	0.42
1:C:501:PRO:O	1:C:504:LYS:HG3	2.19	0.42
1:C:50:TYR:CZ	1:C:53:ILE:HA	2.55	0.42
1:D:433:VAL:HG11	1:D:443:ALA:HB1	2.02	0.42
1:A:137:HIS:HA	1:A:170:GLN:HG3	2.01	0.42
1:A:621:PRO:HG2	3:A:801:UDP:O1A	2.19	0.42
2:F:35:ILE:HG12	2:F:247:HIS:CG	2.55	0.42
1:A:180:LEU:HD21	1:A:492:LEU:HD13	2.02	0.41
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.55	0.41
1:D:658:ASP:OD1	1:D:661:HIS:HB2	2.19	0.41
1:C:463:THR:HG21	1:C:492:LEU:HD23	2.02	0.41
2:E:334:TRP:O	2:E:337:THR:HG22	2.19	0.41
2:H:49:ARG:O	2:H:52:GLU:HG2	2.20	0.41
1:A:706:SER:HB3	1:A:708:LYS:HE2	2.01	0.41
1:B:135:ILE:HD11	1:B:174:ILE:HG21	2.02	0.41
1:B:622:SER:HA	3:B:801:UDP:O3B	2.21	0.41
2:H:42:LYS:HD3	2:H:240:LEU:HD21	2.02	0.41
1:A:425:PRO:HG3	1:A:615:THR:HG22	2.00	0.41
1:C:195:ARG:HD2	1:C:484:LEU:HD11	2.02	0.41
2:F:163:MET:HB3	2:F:189:LEU:HD13	2.03	0.41
1:B:155:TYR:HE1	1:B:209:THR:HG23	1.86	0.41
1:B:285:PHE:O	1:B:289:VAL:HG23	2.20	0.41
1:C:227:LEU:HB2	1:C:460:ALA:HB3	2.03	0.41
1:D:248:VAL:O	1:D:294:GLN:HA	2.21	0.41
2:F:42:LYS:HD3	2:F:240:LEU:HD21	2.01	0.41
1:A:636:GLU:OE1	1:A:678:TYR:OH	2.27	0.41
1:C:135:ILE:HG23	1:C:170:GLN:HB3	2.01	0.41
1:D:439:CYS:SG	3:D:801:UDP:H3'	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:LYS:HB3	1:C:536:ALA:HB2	2.03	0.41
2:F:24:ASN:N	2:F:24:ASN:OD1	2.44	0.41
1:D:23:HIS:CD2	2:G:300:ASN:HD22	2.38	0.41
1:B:323:ARG:O	1:B:329:ARG:NH2	2.54	0.41
1:C:640:GLY:HA2	1:C:668:LEU:HD13	2.02	0.41
1:D:312:GLU:O	1:D:316:LEU:HG	2.20	0.41
1:A:439:CYS:HB2	1:A:441:GLU:OE1	2.21	0.41
1:A:736:ASP:N	1:A:736:ASP:OD1	2.54	0.41
1:B:64:LYS:HE3	1:B:64:LYS:HB3	1.87	0.41
1:C:116:ASP:OD1	1:C:117:ASN:N	2.54	0.41
1:C:679:LEU:HD13	1:C:721:ALA:HB2	2.02	0.41
2:G:31:GLN:HG2	2:G:37:GLU:HB2	2.02	0.41
1:B:696:ASN:OD1	1:B:731:TYR:HB2	2.21	0.41
1:B:98:GLU:HA	1:B:99:PRO:HD3	1.95	0.41
1:C:560:LYS:HE2	1:C:609:HIS:CD2	2.56	0.41
1:D:285:PHE:O	1:D:289:VAL:HG23	2.21	0.41
1:D:317:LEU:HD21	1:D:337:VAL:HG21	2.03	0.41
1:D:319:LEU:HD22	1:D:330:VAL:HG23	2.03	0.41
2:F:201:ASN:HD21	2:F:246:GLN:HG3	1.85	0.41
1:A:552:LEU:HD23	1:A:616:LEU:HD12	2.03	0.41
1:B:226:VAL:HG22	1:B:461:LEU:HD22	2.02	0.41
1:C:317:LEU:HD12	1:C:402:MET:HA	2.03	0.41
2:G:90:SER:HB3	2:G:157:TYR:CE1	2.56	0.41
2:H:299:LEU:HA	2:H:299:LEU:HD12	1.86	0.41
1:C:63:ILE:HG12	1:C:84:LEU:HB3	2.03	0.40
1:C:89:LEU:HD11	1:C:152:GLU:HB3	2.02	0.40
2:E:198:MET:HG3	2:E:272:CYS:SG	2.61	0.40
1:A:619:LEU:HD12	1:A:693:ILE:HG12	2.03	0.40
1:B:544:PHE:CE1	1:B:685:MET:HG2	2.56	0.40
2:E:299:LEU:HA	2:E:299:LEU:HD12	1.97	0.40
2:F:149:ARG:HG2	2:F:282:GLN:OE1	2.21	0.40
2:G:126:ILE:O	2:G:130:VAL:HG22	2.21	0.40
1:B:578:LEU:HD13	1:B:599:TRP:HE3	1.85	0.40
2:E:19:PHE:CE2	2:E:190:LYS:HG2	2.56	0.40
1:A:316:LEU:HA	1:A:319:LEU:HG	2.03	0.40
1:B:116:ASP:OD1	1:B:117:ASN:N	2.54	0.40
1:B:700:ASP:HB3	1:B:703:ARG:HD2	2.04	0.40
1:C:227:LEU:HD23	1:C:435:GLN:HG3	2.02	0.40
2:H:147:GLN:HA	2:H:150:ALA:HB3	2.03	0.40
2:G:196:CYS:O	2:G:200:VAL:HG23	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	732/761 (96%)	712 (97%)	18 (2%)	2 (0%)	46	83
1	B	732/761 (96%)	714 (98%)	16 (2%)	2 (0%)	46	83
1	C	732/761 (96%)	714 (98%)	16 (2%)	2 (0%)	46	83
1	D	731/761 (96%)	711 (97%)	18 (2%)	2 (0%)	46	83
2	E	346/375 (92%)	340 (98%)	6 (2%)	0	100	100
2	F	353/375 (94%)	348 (99%)	5 (1%)	0	100	100
2	G	353/375 (94%)	349 (99%)	4 (1%)	0	100	100
2	H	351/375 (94%)	347 (99%)	4 (1%)	0	100	100
All	All	4330/4544 (95%)	4235 (98%)	87 (2%)	8 (0%)	52	87

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	B	216	ARG
1	C	216	ARG
1	D	216	ARG
1	A	215	VAL
1	D	215	VAL
1	B	215	VAL
1	C	215	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/651 (97%)	627 (100%)	2 (0%)	94	98
1	B	629/651 (97%)	625 (99%)	4 (1%)	90	96
1	C	626/651 (96%)	624 (100%)	2 (0%)	94	98
1	D	627/651 (96%)	625 (100%)	2 (0%)	94	98
2	E	309/340 (91%)	308 (100%)	1 (0%)	94	98
2	F	321/340 (94%)	317 (99%)	4 (1%)	78	92
2	G	315/340 (93%)	313 (99%)	2 (1%)	90	96
2	H	315/340 (93%)	314 (100%)	1 (0%)	94	98
All	All	3771/3964 (95%)	3753 (100%)	18 (0%)	92	96

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	THR
1	A	620	MET
1	B	4	ASN
1	B	17	ILE
1	B	219	THR
1	B	620	MET
1	C	17	ILE
1	C	620	MET
1	D	17	ILE
1	D	620	MET
2	E	208	PHE
2	F	7	GLN
2	F	127	ARG
2	F	183	THR
2	F	208	PHE
2	G	208	PHE
2	G	322	ASP
2	H	208	PHE

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

Mol	Chain	Res	Type
1	B	34	HIS
1	B	450	ASN
2	F	201	ASN
2	G	80	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\# Z > 2$
3	UDP	A	801	-	20,26,26	0.82	0	24,40,40	1.58	1 (4%)
4	DTP	A	802	5	25,32,32	0.92	1 (4%)	26,50,50	1.80	3 (11%)
4	DTP	A	804	5	25,32,32	0.97	1 (4%)	26,50,50	1.64	2 (7%)
4	DTP	A	805	5	25,32,32	0.90	1 (4%)	26,50,50	1.64	1 (3%)
3	UDP	B	801	-	20,26,26	0.87	0	24,40,40	1.60	1 (4%)
4	DTP	B	802	5	25,32,32	0.91	1 (4%)	26,50,50	1.63	3 (11%)
4	DTP	B	804	5	25,32,32	0.97	1 (4%)	26,50,50	1.58	1 (3%)
4	DTP	B	805	5	25,32,32	0.91	1 (4%)	26,50,50	1.65	1 (3%)
3	UDP	C	801	-	20,26,26	0.84	0	24,40,40	1.64	1 (4%)
4	DTP	C	802	5	25,32,32	0.91	1 (4%)	26,50,50	1.62	2 (7%)
4	DTP	C	804	5	25,32,32	0.96	1 (4%)	26,50,50	1.65	1 (3%)
4	DTP	C	805	5	25,32,32	0.92	1 (4%)	26,50,50	1.59	1 (3%)
3	UDP	D	801	-	20,26,26	0.83	0	24,40,40	1.57	1 (4%)
4	DTP	D	802	5	25,32,32	0.90	1 (4%)	26,50,50	1.79	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DTP	D	804	5	25,32,32	0.97	1 (4%)	26,50,50	1.54	1 (3%)
4	DTP	D	805	5	25,32,32	0.90	1 (4%)	26,50,50	1.65	1 (3%)
6	FEO	E	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-
6	FEO	F	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-
6	FEO	G	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-
6	FEO	H	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-

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
3	UDP	A	801	-	-	0/12/32/32	0/2/2/2
4	DTP	A	802	5	-	0/18/34/34	0/3/3/3
4	DTP	A	804	5	-	0/18/34/34	0/3/3/3
4	DTP	A	805	5	-	0/18/34/34	0/3/3/3
3	UDP	B	801	-	-	0/12/32/32	0/2/2/2
4	DTP	B	802	5	-	0/18/34/34	0/3/3/3
4	DTP	B	804	5	-	0/18/34/34	0/3/3/3
4	DTP	B	805	5	-	0/18/34/34	0/3/3/3
3	UDP	C	801	-	-	0/12/32/32	0/2/2/2
4	DTP	C	802	5	-	0/18/34/34	0/3/3/3
4	DTP	C	804	5	-	0/18/34/34	0/3/3/3
4	DTP	C	805	5	-	0/18/34/34	0/3/3/3
3	UDP	D	801	-	-	0/12/32/32	0/2/2/2
4	DTP	D	802	5	-	0/18/34/34	0/3/3/3
4	DTP	D	804	5	-	0/18/34/34	0/3/3/3
4	DTP	D	805	5	-	0/18/34/34	0/3/3/3
6	FEO	E	501	2,7	-	0/0/0/0	0/0/0/0
6	FEO	F	501	2,7	-	0/0/0/0	0/0/0/0
6	FEO	G	501	2,7	-	0/0/0/0	0/0/0/0
6	FEO	H	501	2,7	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	802	DTP	C5-C4	2.98	1.47	1.40
4	A	805	DTP	C5-C4	3.02	1.47	1.40
4	B	802	DTP	C5-C4	3.06	1.47	1.40
4	D	805	DTP	C5-C4	3.06	1.47	1.40
4	B	805	DTP	C5-C4	3.06	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	802	DTP	C5-C4	3.07	1.47	1.40
4	C	805	DTP	C5-C4	3.11	1.47	1.40
4	A	802	DTP	C5-C4	3.11	1.47	1.40
4	B	804	DTP	C5-C4	3.28	1.47	1.40
4	C	804	DTP	C5-C4	3.28	1.47	1.40
4	A	804	DTP	C5-C4	3.33	1.48	1.40
4	D	804	DTP	C5-C4	3.35	1.48	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	802	DTP	N3-C2-N1	-7.03	123.35	128.87
4	A	802	DTP	N3-C2-N1	-6.78	123.55	128.87
4	C	804	DTP	N3-C2-N1	-6.77	123.55	128.87
4	B	805	DTP	N3-C2-N1	-6.74	123.58	128.87
4	A	804	DTP	N3-C2-N1	-6.73	123.58	128.87
4	C	802	DTP	N3-C2-N1	-6.68	123.62	128.87
4	B	802	DTP	N3-C2-N1	-6.67	123.63	128.87
4	A	805	DTP	N3-C2-N1	-6.58	123.70	128.87
4	D	805	DTP	N3-C2-N1	-6.57	123.71	128.87
4	C	805	DTP	N3-C2-N1	-6.57	123.71	128.87
4	B	804	DTP	N3-C2-N1	-6.32	123.91	128.87
4	D	804	DTP	N3-C2-N1	-6.29	123.93	128.87
4	D	802	DTP	C1'-N9-C4	-2.28	123.74	127.07
4	A	802	DTP	C1'-N9-C4	-2.06	124.06	127.07
4	B	802	DTP	C2'-C3'-C4'	2.04	106.91	102.77
4	C	802	DTP	O3G-PG-O2G	2.10	115.16	107.44
4	B	802	DTP	O3G-PG-O2G	2.11	115.21	107.44
4	A	802	DTP	O4'-C1'-N9	2.35	111.82	107.71
4	A	804	DTP	O3G-PG-O2G	2.37	116.14	107.44
3	A	801	UDP	C4-N3-C2	5.89	120.41	114.21
3	B	801	UDP	C4-N3-C2	5.90	120.42	114.21
3	D	801	UDP	C4-N3-C2	6.00	120.53	114.21
3	C	801	UDP	C4-N3-C2	6.39	120.94	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	UDP	2	0
4	A	802	DTP	1	0
4	A	804	DTP	1	0
3	B	801	UDP	3	0
4	B	802	DTP	3	0
4	B	805	DTP	1	0
3	C	801	UDP	3	0
4	C	804	DTP	1	0
3	D	801	UDP	2	0
4	D	802	DTP	1	0
4	D	804	DTP	1	0
4	D	805	DTP	1	0
6	G	501	FEO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	734/761 (96%)	-0.22	4 (0%) 91 88	55, 67, 97, 116	0
1	B	734/761 (96%)	-0.15	2 (0%) 94 93	56, 72, 86, 103	0
1	C	734/761 (96%)	0.30	27 (3%) 45 35	85, 102, 112, 118	0
1	D	733/761 (96%)	-0.03	6 (0%) 87 82	68, 83, 101, 110	0
2	E	350/375 (93%)	0.13	6 (1%) 73 64	74, 94, 106, 123	0
2	F	357/375 (95%)	-0.33	1 (0%) 94 93	48, 61, 80, 99	0
2	G	357/375 (95%)	-0.29	0 100 100	49, 63, 86, 103	0
2	H	355/375 (94%)	-0.05	6 (1%) 73 64	69, 80, 102, 116	0
All	All	4354/4544 (95%)	-0.06	52 (1%) 81 72	48, 78, 106, 123	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	166	TYR	4.2
1	C	128	PHE	3.9
1	C	379	TYR	3.7
2	H	363	SER	3.6
2	E	170	LEU	3.2
1	C	81	ALA	3.2
1	C	105	HIS	3.0
1	D	49	PHE	3.0
1	A	14	THR	2.9
1	C	123	TYR	2.9
1	C	131	MET	2.9
1	C	375	PHE	2.8
1	C	364	LEU	2.7
1	C	706	SER	2.6
1	C	382	TYR	2.5
1	D	388	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	708	LYS	2.5
1	C	347	LEU	2.5
1	C	361	VAL	2.5
1	C	120	LEU	2.4
1	C	380	THR	2.4
1	C	100	PRO	2.4
1	D	48	GLN	2.4
1	C	225	CYS	2.4
1	C	137	HIS	2.4
1	C	58	ILE	2.4
1	C	97	PHE	2.4
2	H	183	THR	2.4
1	C	68	ASP	2.3
1	C	692	SER	2.3
1	D	224	SER	2.3
1	C	437	ASN	2.2
2	H	182	VAL	2.2
1	C	356	PHE	2.2
1	A	4	ASN	2.2
1	A	10	ARG	2.2
2	H	361	ILE	2.2
1	A	6	LEU	2.2
2	E	1	ALA	2.2
2	E	19	PHE	2.2
2	H	179	GLY	2.1
2	F	341	SER	2.1
1	B	48	GLN	2.1
2	H	362	ASP	2.1
1	C	362	PRO	2.1
1	C	378	LEU	2.1
1	B	102	LEU	2.1
2	E	114	SER	2.1
1	C	103	TYR	2.0
2	E	138	ASP	2.0
1	D	387	SER	2.0
1	D	456	ASN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	UDP	D	801	25/25	0.96	0.30	0.72	75,80,84,87	0
3	UDP	C	801	25/25	0.93	0.34	0.56	94,97,99,99	0
3	UDP	B	801	25/25	0.96	0.28	0.51	64,67,70,71	0
3	UDP	A	801	25/25	0.96	0.18	-0.16	62,67,70,71	0
4	DTP	C	804	30/30	0.91	0.26	-0.69	112,116,121,125	0
4	DTP	D	802	30/30	0.92	0.22	-0.87	90,95,101,102	0
4	DTP	C	805	30/30	0.97	0.16	-1.20	91,93,95,96	0
4	DTP	B	805	30/30	0.96	0.15	-1.26	65,67,71,74	0
4	DTP	D	805	30/30	0.96	0.14	-1.32	85,88,91,94	0
4	DTP	B	802	30/30	0.97	0.18	-1.37	77,79,85,86	0
4	DTP	C	802	30/30	0.93	0.18	-1.46	105,107,118,120	0
4	DTP	A	802	30/30	0.93	0.21	-1.57	91,100,107,112	0
6	FEO	H	501	3/3	0.99	0.17	-1.59	72,72,72,72	0
4	DTP	A	805	30/30	0.98	0.12	-1.64	56,58,63,64	0
4	DTP	D	804	30/30	0.93	0.17	-1.70	95,103,111,115	0
6	FEO	G	501	3/3	0.99	0.15	-1.74	51,51,52,53	0
4	DTP	A	804	30/30	0.92	0.21	-1.83	96,105,116,118	0
6	FEO	F	501	3/3	0.98	0.14	-1.95	51,51,52,55	0
4	DTP	B	804	30/30	0.92	0.18	-2.28	83,90,95,96	0
6	FEO	E	501	3/3	0.96	0.15	-2.50	83,83,86,93	0
5	MG	A	806	1/1	0.98	0.05	-	57,57,57,57	0
5	MG	C	806	1/1	0.93	0.13	-	94,94,94,94	0
5	MG	D	803	1/1	0.93	0.05	-	104,104,104,104	0
5	MG	C	803	1/1	0.95	0.05	-	117,117,117,117	0
5	MG	B	806	1/1	0.94	0.12	-	67,67,67,67	0
5	MG	A	803	1/1	0.91	0.07	-	104,104,104,104	0
5	MG	D	806	1/1	0.96	0.06	-	87,87,87,87	0
5	MG	B	803	1/1	0.97	0.04	-	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.