Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:18 AM GMT

PDB ID	:	3A8I
Title	:	Crystal Structure of ET-EHred-5-CH3-THF complex
Authors	:	Okamura-Ikeda, K.; Hosaka, H.
Deposited on	:	2009-10-06
Resolution	:	1.99 Å(reported)

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.99 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.
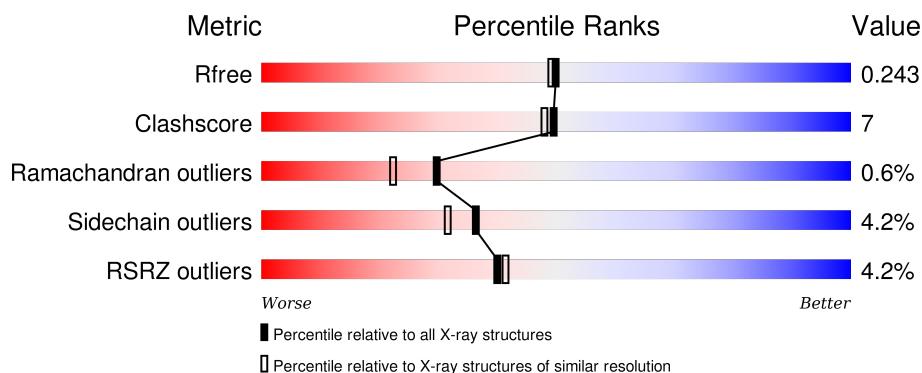
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	364	4% 81% 17% •
1	B	364	3% 83% 15% •
1	C	364	3% 82% 15% •
1	D	364	4% 80% 18% •
2	E	129	10% 81% 16% • • •

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Mol	Chain	Length	Quality of chain
2	F	129	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14524 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 Aminomethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total 2815	C 1777	N 492	O 531	S 15	0	0	0
1	B	363	Total 2865	C 1807	N 502	O 541	S 15	0	7	0
1	C	363	Total 2815	C 1777	N 492	O 531	S 15	0	0	0
1	D	363	Total 2815	C 1777	N 492	O 531	S 15	0	0	0

- Molecule 2 is a protein called Glycine cleavage system H protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	128	Total 974	C 611	N 147	O 212	S 4	0	0	0
2	F	128	Total 974	C 611	N 147	O 212	S 4	0	0	0

- Molecule 3 is 5-METHYL-5,6,7,8-TETRAHYDROFOLIC ACID (three-letter code: C2F) (formula: $C_{20}H_{25}N_7O_6$).
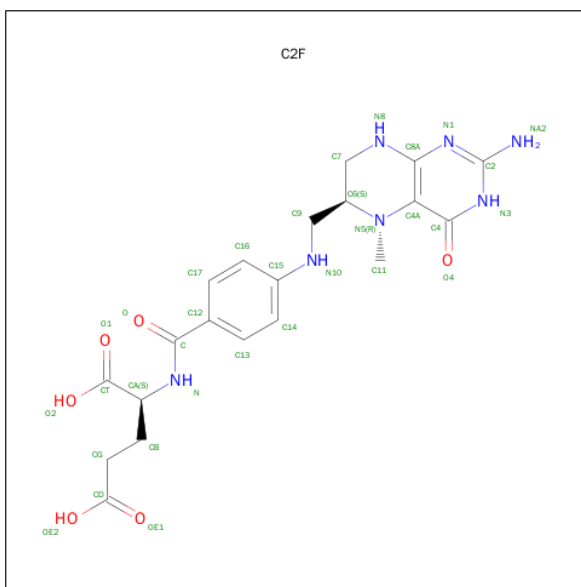
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 33	C 20	N 7	O 6	0	0
3	B	1	Total 33	C 20	N 7	O 6	0	0
3	C	1	Total 33	C 20	N 7	O 6	0	0
3	D	1	Total 33	C 20	N 7	O 6	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
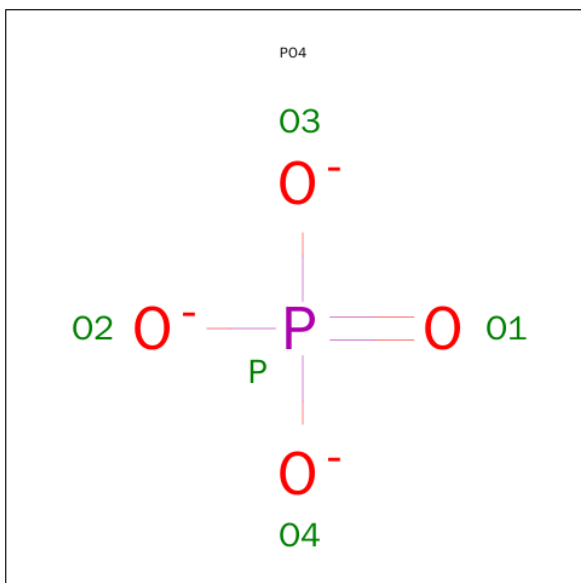
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 5	O 4	P 1	0	0
4	D	1	Total 5	O 4	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total 282	O 282	0	0
5	B	251	Total 251	O 251	0	0
5	C	249	Total 249	O 249	0	0
5	D	246	Total 246	O 246	0	0
5	E	61	Total 61	O 61	0	0
5	F	35	Total 35	O 35	0	0

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: Aminomethyltransferase

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N358 V362 A363

• Molecule 1: Aminomethyltransferase

Chain D:

4%

80% 18%

MET A1 G44 I53 R57 R62 A82 I95 D96 D97 V100 Y101 D106 F107 F108 R109 S114 E118 K119 D120 W123 E129 P130 I133 M143 I144 A145 V146 A151 Q152 F159 Q163 R164 F182 T186 G193 Y194 E195 I196 A197

L198 R208 A209 K216 Y235 E238 M239 D240 E241 R266 E267 A268 L269 E274 H275 V284 R292 N293 E294 L295 T300 D301 A302 Q303 G304 N305 Q306 H307 E308 G309 S313 F316 S317 P318 I324 V329 P330 I338 V339 R342 N343 R344 E345 K349

V350 T351 V356 R357 N358 G359 V362 A363

• Molecule 2: Glycine cleavage system H protein

Chain E:

10%

81% 16%

MET S1 N2 A5 S10 K11 E12 H13 L16 A20 D21 Y24 T25 V26 G27 H31 L35 D38 M39 V42 E46 V47 G48 K64 S85 I101 E109 S110 L115 L116 D117 A118 T119 L124 L125 E126 D127 E128

• Molecule 2: Glycine cleavage system H protein

Chain F:

7%

73% 25%

MET S1 N2 V3 P4 A5 E6 L7 K8 Y9 S10 K11 E12 L16 R17 K18 E19 A20 D21 G22 T23 Y24 T25 I28 T29 E30 Q33 E34 M39 V42 V47 S52 D56 A60 E61 D68 I69 A83 S87 V91 K105 S110 L115 L116

T119 A120 A123 E126 D127 E128

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.98Å 88.93Å 97.99Å 91.53° 102.47° 89.59°	Depositor
Resolution (Å)	29.77 – 1.99 29.77 – 1.99	Depositor EDS
% Data completeness (in resolution range)	84.4 (29.77-1.99) 84.0 (29.77-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.182 , 0.244 0.182 , 0.243	Depositor DCC
R_{free} test set	5115 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	EDS
Estimated twinning fraction	0.148 for -h,k,-l	Xtriage
L-test for twinning [2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.32$	Xtriage
Outliers	0 of 102296 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14524	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: PO4, C2F, LA2

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	1.16	4/2873 (0.1%)	1.02	12/3891 (0.3%)
1	B	1.12	3/2928 (0.1%)	0.99	8/3967 (0.2%)
1	C	1.15	5/2873 (0.2%)	0.98	6/3891 (0.2%)
1	D	1.15	3/2873 (0.1%)	1.02	11/3891 (0.3%)
2	E	0.96	0/970	0.93	3/1321 (0.2%)
2	F	0.91	0/970	0.88	1/1321 (0.1%)
All	All	1.12	15/13487 (0.1%)	0.99	41/18282 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	238	GLU	CB-CG	7.43	1.66	1.52
1	C	241	GLU	CB-CG	6.09	1.63	1.52
1	A	118	GLU	CB-CG	5.73	1.63	1.52
1	C	2	GLN	CB-CG	-5.71	1.37	1.52
1	D	144	ILE	CB-CG2	5.69	1.70	1.52
1	D	118	GLU	CG-CD	5.63	1.60	1.51
1	B	90	ALA	CA-CB	5.47	1.64	1.52
1	C	235	TYR	CD2-CE2	5.47	1.47	1.39
1	A	118	GLU	CG-CD	5.43	1.60	1.51
1	B	122	SER	CB-OG	-5.39	1.35	1.42
1	A	34	ASP	CB-CG	-5.17	1.40	1.51
1	B	146	VAL	CB-CG1	5.17	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	GLU	CB-CG	5.13	1.61	1.52
1	C	235	TYR	CD1-CE1	5.10	1.47	1.39
1	A	108	PHE	CE1-CZ	5.06	1.47	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH1	12.93	126.76	120.30
1	D	266	ARG	NE-CZ-NH2	-12.58	114.01	120.30
2	E	35	LEU	CA-CB-CG	9.30	136.70	115.30
1	D	266	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	B	208	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	C	72	ASP	CB-CG-OD1	7.20	124.78	118.30
1	D	97	ASP	CB-CG-OD1	7.15	124.74	118.30
1	D	109	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	62	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	34	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	A	97	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	D	208	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	97	ASP	CB-CG-OD1	6.65	124.28	118.30
1	D	266	ARG	CG-CD-NE	-6.48	98.19	111.80
1	A	227	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	F	16	LEU	CA-CB-CG	6.23	129.63	115.30
1	D	62	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	109	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	97	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	117	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	E	11	LYS	N-CA-C	5.70	126.39	111.00
1	C	133	ILE	CB-CA-C	-5.59	100.42	111.60
1	D	208	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	140	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	109	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	295	LEU	CB-CG-CD1	5.50	120.34	111.00
1	C	97	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	227	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	47	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	62	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	62	ARG	CD-NE-CZ	5.37	131.12	123.60
1	D	301	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	171	LYS	CD-CE-NZ	-5.32	99.46	111.70
1	B	47	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	266	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	120	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	34	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	B	208	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	180	ASP	CB-CG-OD1	5.09	122.88	118.30
2	E	35	LEU	CB-CG-CD2	5.03	119.55	111.00
1	D	266	ARG	CD-NE-CZ	5.02	130.63	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	292	ARG	Peptide

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	2815	0	2771	36	0
1	B	2865	0	2818	37	0
1	C	2815	0	2771	42	0
1	D	2815	0	2771	35	0
2	E	974	0	922	16	0
2	F	974	0	923	22	0
3	A	33	0	23	1	0
3	B	33	0	23	2	0
3	C	33	0	23	1	0
3	D	33	0	23	2	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
5	A	282	0	0	4	0
5	B	251	0	0	5	0
5	C	249	0	0	7	1
5	D	246	0	0	2	1
5	E	61	0	0	2	0
5	F	35	0	0	2	0
All	All	14524	0	13068	187	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:HH11	1:C:266:ARG:HG3	1.16	1.10
1:C:298:ARG:HB2	1:C:338:ILE:CD1	2.01	0.91
2:F:11:LYS:HG3	2:F:12:GLU:OE2	1.75	0.85
1:C:292:ARG:H	1:C:295:LEU:HD22	1.43	0.83
2:F:116:LEU:HD23	2:F:120:ALA:HB1	1.60	0.83
1:C:128:ALA:HB1	1:C:133:ILE:HG13	1.61	0.82
1:C:298:ARG:HB2	1:C:338:ILE:HD11	1.63	0.80
1:D:357:ARG:O	1:D:359:GLY:N	2.13	0.80
1:A:4:THR:HG23	5:A:692:HOH:O	1.82	0.79
1:B:344:ARG:NH1	5:B:739:HOH:O	2.16	0.78
1:B:78:LYS:HE2	1:B:174:PHE:HZ	1.49	0.77
1:C:266:ARG:HG3	1:C:266:ARG:NH1	1.91	0.77
1:D:300:THR:O	1:D:305:ASN:O	2.02	0.77
1:C:267:GLU:HG3	5:C:607:HOH:O	1.86	0.75
1:D:119:LYS:HD2	5:D:756:HOH:O	1.85	0.75
1:B:4[A]:THR:O	1:B:7:TYR:HB2	1.88	0.71
1:D:292:ARG:H	1:D:295:LEU:HD22	1.54	0.71
1:C:146:VAL:HG12	1:C:151:ALA:HB1	1.72	0.70
1:B:78:LYS:HD3	5:B:626:HOH:O	1.89	0.70
2:F:56:ASP:OD1	2:F:68:ASP:HB3	1.90	0.69
1:C:340:GLN:NE2	1:C:342:ARG:O	2.21	0.69
1:C:338:ILE:HG13	1:C:345:GLU:HB3	1.74	0.69
2:F:61:GLU:OE1	5:F:227:HOH:O	2.11	0.69
1:A:341:ILE:HD12	1:A:346:MET:HG3	1.72	0.69
1:B:2[B]:GLN:HB2	1:B:23:TRP:CE3	2.27	0.68
2:F:39:MET:CE	2:F:60:ALA:HB1	2.24	0.67
2:E:27:GLY:HA2	2:E:101:ILE:HG12	1.76	0.67
1:A:23:TRP:CE3	1:A:50:HIS:HB3	2.29	0.67
2:E:46:GLU:OE1	5:E:260:HOH:O	2.13	0.67
1:C:357:ARG:HG2	5:C:755:HOH:O	1.94	0.66
1:B:23:TRP:CZ3	1:B:50[A]:HIS:CE1	2.84	0.66
2:E:31:HIS:ND1	5:E:212:HOH:O	2.28	0.66
1:A:302:ALA:HB3	1:A:303:GLN:HE22	1.60	0.66
1:A:2:GLN:HG3	5:A:637:HOH:O	1.96	0.64
2:F:23:THR:HG22	2:F:105:LYS:HB2	1.78	0.64
1:D:284:VAL:HG22	1:D:324:ILE:HG22	1.80	0.63
2:E:10:SER:OG	2:E:12:GLU:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:SER:HA	1:B:106:ASP:OD1	1.98	0.63
1:D:146:VAL:HG12	1:D:151:ALA:HB1	1.80	0.63
1:B:171:LYS:NZ	2:E:85:SER:O	2.31	0.62
2:F:39:MET:HE2	2:F:60:ALA:HB1	1.80	0.62
1:C:271:VAL:HB	5:C:710:HOH:O	1.99	0.62
1:C:57:ARG:NH2	5:C:819:HOH:O	2.33	0.61
1:D:338:ILE:HG21	1:D:345:GLU:HG3	1.82	0.60
1:B:2[B]:GLN:HB2	1:B:23:TRP:CZ3	2.37	0.60
2:F:30:GLU:O	2:F:33:GLN:HG3	2.00	0.60
1:D:267:GLU:HG3	5:D:603:HOH:O	2.01	0.60
1:A:146:VAL:HG12	1:A:151:ALA:HB1	1.83	0.59
1:C:37:HIS:NE2	5:C:704:HOH:O	2.32	0.59
1:C:316:PHE:O	1:C:318:PRO:HD3	2.03	0.58
1:A:302:ALA:HB3	1:A:303:GLN:NE2	2.18	0.58
1:D:316:PHE:O	1:D:318:PRO:HD3	2.02	0.58
2:F:8:LYS:HB2	2:F:16:LEU:HB2	1.85	0.57
1:A:123:TRP:O	1:A:127:HIS:HD2	1.89	0.56
1:B:23:TRP:HZ2	1:D:129:GLU:OE2	1.87	0.56
1:C:279:LYS:NZ	1:C:333:ILE:HG22	2.21	0.56
1:C:338:ILE:HD13	1:C:338:ILE:O	2.07	0.55
1:C:307:HIS:HB3	1:C:330:PRO:HG2	1.87	0.55
2:F:60:ALA:HB2	2:F:69:ILE:HD11	1.88	0.55
1:B:302:ALA:HB3	1:B:303:GLN:OE1	2.08	0.54
1:D:186:THR:O	1:D:195:GLU:HG3	2.07	0.54
1:C:320:LEU:HB3	1:C:322:TYR:CZ	2.42	0.54
2:E:11:LYS:HA	2:E:13:HIS:H	1.73	0.53
1:C:256:TRP:O	1:C:266:ARG:NH2	2.40	0.53
1:A:128:ALA:HB3	1:A:135:ILE:HD11	1.90	0.53
1:D:53:ILE:HD11	1:D:143:MET:HE2	1.91	0.53
1:D:182:PHE:HB3	1:D:197:ALA:HB3	1.91	0.53
2:F:28:ILE:HD11	2:F:91:VAL:CG1	2.39	0.53
1:C:143:MET:HE2	5:C:612:HOH:O	2.08	0.53
1:B:128:ALA:HB3	1:B:135:ILE:HD11	1.91	0.53
1:D:159:PHE:O	1:D:164:ARG:NH1	2.42	0.52
1:B:78:LYS:HE2	1:B:174:PHE:CZ	2.37	0.52
1:A:34:ASP:HB3	1:A:216:LYS:HZ1	1.74	0.52
1:D:349:LYS:HE3	1:D:351:THR:HG22	1.92	0.52
2:F:52:SER:HB2	5:F:225:HOH:O	2.10	0.52
1:A:338:ILE:CG2	1:A:345:GLU:HB3	2.39	0.51
1:B:284:VAL:HG13	1:B:322:TYR:CE1	2.45	0.51
1:D:238:GLU:OE2	1:D:313:SER:OG	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MET:CE	1:A:143:MET:HE2	2.41	0.50
1:C:10:HIS:CE1	1:C:47:ASP:HB2	2.47	0.50
1:A:269:LEU:HD12	1:A:272:GLN:NE2	2.26	0.49
1:B:216:LYS:NZ	5:B:746:HOH:O	2.45	0.49
1:D:159:PHE:HB3	1:D:163:GLN:HB2	1.93	0.49
1:C:180:ASP:OD2	1:C:202:LYS:HD3	2.13	0.49
1:C:171:LYS:HA	5:C:639:HOH:O	2.13	0.49
1:D:356:VAL:HG12	1:D:357:ARG:N	2.28	0.49
2:F:39:MET:CE	2:F:42:VAL:HG22	2.43	0.49
1:C:279:LYS:HZ1	1:C:333:ILE:HG22	1.78	0.48
1:A:338:ILE:HG21	1:A:345:GLU:HB3	1.94	0.48
1:A:7:TYR:O	1:A:11:THR:HG23	2.12	0.48
2:F:1:SER:O	2:F:3:VAL:N	2.44	0.48
1:B:139:ASP:HB2	1:D:133:ILE:O	2.13	0.48
2:E:10:SER:OG	2:E:11:LYS:N	2.46	0.48
1:D:307:HIS:HB3	1:D:330:PRO:HG2	1.95	0.48
2:F:18:LYS:HE3	2:F:22:GLY:HA2	1.95	0.48
2:F:16:LEU:HG	2:F:115:LEU:HD13	1.96	0.48
1:C:284:VAL:HG13	1:C:322:TYR:CE1	2.49	0.48
1:A:12:LEU:O	1:A:12:LEU:HD12	2.14	0.47
1:B:2[B]:GLN:CB	1:B:23:TRP:CZ3	2.97	0.47
1:C:180:ASP:OD2	1:C:202:LYS:CD	2.62	0.47
1:B:3[A]:GLN:HG3	1:B:7:TYR:CG	2.50	0.47
2:F:39:MET:HE1	2:F:42:VAL:HG22	1.97	0.47
1:A:4:THR:HG22	1:A:23:TRP:CE3	2.49	0.47
1:B:119:LYS:HD2	1:B:241:GLU:OE2	2.15	0.46
1:A:33:ILE:HG12	2:E:38:ASP:OD2	2.15	0.46
2:E:39:MET:CE	2:E:42:VAL:HB	2.45	0.46
1:B:31:SER:HB3	1:B:34:ASP:HB2	1.98	0.46
2:F:120:ALA:O	2:F:123:ALA:HB3	2.16	0.46
1:D:44:GLY:HA2	1:D:216:LYS:O	2.16	0.46
1:A:270:GLU:O	1:A:274:GLU:HG3	2.16	0.46
1:C:64:PHE:CZ	1:C:128:ALA:HB2	2.51	0.46
1:B:118:GLU:OE1	5:B:835:HOH:O	2.20	0.46
1:A:286:THR:HA	1:A:322:TYR:CD1	2.51	0.46
1:C:227:ARG:HD2	1:C:227:ARG:C	2.36	0.45
1:B:270:GLU:O	1:B:274:GLU:HG3	2.16	0.45
1:C:235:TYR:CZ	1:C:240:ASP:HA	2.51	0.45
1:B:4[B]:THR:CB	1:B:5[B]:PRO:CD	2.95	0.45
1:C:259:ALA:HA	1:C:266:ARG:HH21	1.81	0.45
1:C:159:PHE:HB3	1:C:163:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:16:LEU:HA	2:E:25:THR:O	2.16	0.45
1:A:35:GLU:HG3	1:A:216:LYS:HZ3	1.82	0.45
3:D:401:C2F:H92	3:D:401:C2F:H16	1.47	0.45
1:A:71:ASN:OD1	1:A:75:LYS:CE	2.64	0.45
1:B:352:LYS:HE3	2:E:48:GLY:O	2.17	0.45
2:E:10:SER:OG	2:E:12:GLU:CB	2.64	0.44
3:D:401:C2F:H92	3:D:401:C2F:C8A	2.46	0.44
1:A:34:ASP:HB3	1:A:216:LYS:NZ	2.32	0.44
1:D:152:GLN:HE21	1:D:193:GLY:H	1.65	0.44
1:D:57:ARG:HA	1:D:106:ASP:O	2.17	0.44
1:D:82:ALA:HB2	1:D:101:TYR:CD2	2.52	0.44
1:A:70:ALA:HB1	1:A:254:ILE:HD12	1.99	0.44
1:C:298:ARG:HB2	1:C:338:ILE:HD12	1.94	0.44
1:C:293:ASN:O	1:C:294:GLU:HB2	2.17	0.44
1:C:311:ILE:HG23	1:C:325:ALA:HB1	1.99	0.44
1:B:36:HIS:CE1	1:B:229:GLU:OE1	2.70	0.44
1:A:2:GLN:HB2	1:A:23:TRP:CD1	2.53	0.43
1:A:15:ALA:HB1	1:A:26:PRO:HB3	2.00	0.43
1:B:170:MET:HE1	1:B:176:VAL:HG12	1.99	0.43
1:A:198:LEU:N	1:A:198:LEU:HD23	2.34	0.43
1:B:202:LYS:HE3	5:B:833:HOH:O	2.18	0.43
5:A:882:HOH:O	2:E:64:LA2:S8	2.37	0.43
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.73	0.43
1:C:338:ILE:CG1	1:C:345:GLU:HB3	2.47	0.43
1:A:60:ARG:HB2	5:A:765:HOH:O	2.19	0.43
2:E:16:LEU:HG	2:E:26:VAL:HG22	2.00	0.43
1:B:146:VAL:HG12	1:B:151:ALA:HB1	2.01	0.43
1:B:303:GLN:CD	1:B:303:GLN:H	2.23	0.42
1:D:95:ILE:HD13	1:D:123:TRP:CE2	2.54	0.42
1:A:128:ALA:CB	1:A:135:ILE:HD11	2.49	0.42
1:D:114:SER:OG	4:D:501:PO4:O4	2.33	0.42
1:D:57:ARG:HG2	1:D:107:PHE:CD1	2.54	0.42
1:C:338:ILE:HD13	1:C:338:ILE:C	2.40	0.42
2:F:116:LEU:HD23	2:F:120:ALA:CB	2.38	0.42
1:D:95:ILE:CD1	1:D:123:TRP:CE2	3.03	0.42
3:A:401:C2F:H92	3:A:401:C2F:H16	1.55	0.42
1:A:299:PHE:CE2	1:A:333:ILE:HA	2.54	0.42
1:B:4[B]:THR:HB	1:B:5[B]:PRO:HD3	2.01	0.42
1:A:96:ASP:OD2	1:A:120:ASP:OD2	2.38	0.42
2:E:117:ASP:O	2:E:118:ALA:C	2.59	0.42
1:D:293:ASN:N	1:D:293:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5[B]:PRO:HG2	1:B:142:SER:OG	2.20	0.41
1:B:6:LEU:O	1:B:7:TYR:C	2.59	0.41
1:A:31:SER:OG	1:A:34:ASP:HB2	2.20	0.41
1:C:341:ILE:HD12	1:C:346:MET:HG3	2.00	0.41
1:A:35:GLU:HG3	1:A:216:LYS:NZ	2.36	0.41
1:B:170:MET:CE	1:B:176:VAL:HG12	2.50	0.41
1:A:57:ARG:HA	1:A:106:ASP:O	2.20	0.41
2:F:83:ALA:O	2:F:87:SER:HB2	2.20	0.41
1:C:284:VAL:HG13	1:C:322:TYR:CD1	2.55	0.41
1:B:299:PHE:CD1	1:B:333:ILE:HG13	2.55	0.41
3:C:401:C2F:H16	3:C:401:C2F:H92	1.44	0.41
1:B:23:TRP:CE3	1:B:50[A]:HIS:CE1	3.09	0.41
1:A:139:ASP:HB2	1:C:133:ILE:O	2.21	0.41
2:E:16:LEU:HD13	2:E:115:LEU:HD13	2.03	0.41
1:C:254:ILE:HD12	1:C:269:LEU:HD21	2.02	0.41
1:D:235:TYR:CZ	1:D:240:ASP:HA	2.56	0.41
1:C:129:GLU:HB3	1:C:130:PRO:HD3	2.03	0.41
1:D:292:ARG:CG	1:D:293:ASN:N	2.84	0.40
1:D:129:GLU:HB3	1:D:130:PRO:HD3	2.03	0.40
1:B:57:ARG:HA	1:B:106:ASP:O	2.21	0.40
1:D:309:GLY:HA3	1:D:329:VAL:HG12	2.02	0.40
1:B:357:ARG:HH22	3:B:401:C2F:CT	2.34	0.40
2:F:4:PRO:HD2	2:F:9:TYR:OH	2.21	0.40
3:B:401:C2F:H92	3:B:401:C2F:H16	1.78	0.40
1:D:292:ARG:HG3	1:D:293:ASN:N	2.35	0.40
1:D:198:LEU:HD23	1:D:198:LEU:N	2.37	0.40
2:F:19:GLU:OE2	2:F:25:THR:OG1	2.24	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:849:HOH:O	5:D:699:HOH:O[1_656]	2.01	0.19

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	361/364 (99%)	347 (96%)	11 (3%)	3 (1%)	24	15
1	B	367/364 (101%)	353 (96%)	9 (2%)	5 (1%)	14	6
1	C	361/364 (99%)	350 (97%)	10 (3%)	1 (0%)	46	41
1	D	361/364 (99%)	346 (96%)	13 (4%)	2 (1%)	30	22
2	E	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
2	F	125/129 (97%)	118 (94%)	6 (5%)	1 (1%)	24	15
All	All	1700/1714 (99%)	1633 (96%)	55 (3%)	12 (1%)	30	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	GLU
1	D	358	ASN
2	F	20	ALA
1	C	293	ASN
1	A	278	GLU
1	B	276	GLY
1	D	359	GLY
1	A	42	ASP
1	B	2[A]	GLN
1	B	2[B]	GLN
1	B	42	ASP
1	A	342	ARG

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	291/292 (100%)	279 (96%)	12 (4%)	37	32
1	B	297/292 (102%)	286 (96%)	11 (4%)	41	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	291/292 (100%)	278 (96%)	13 (4%)	34	29
1	D	291/292 (100%)	279 (96%)	12 (4%)	37	32
2	E	102/103 (99%)	96 (94%)	6 (6%)	24	18
2	F	102/103 (99%)	99 (97%)	3 (3%)	50	49
All	All	1374/1374 (100%)	1317 (96%)	57 (4%)	36	32

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	GLU
1	A	34	ASP
1	A	79	SER
1	A	100	VAL
1	A	205	ASP
1	A	239	MET
1	A	295	LEU
1	A	342	ARG
1	A	343	ASN
1	A	360	LYS
1	A	362	VAL
1	B	12	LEU
1	B	34	ASP
1	B	79	SER
1	B	100	VAL
1	B	205	ASP
1	B	239	MET
1	B	273	ARG
1	B	288	LYS
1	B	306	GLN
1	B	340	GLN
1	B	352	LYS
1	C	100	VAL
1	C	133	ILE
1	C	180	ASP
1	C	198	LEU
1	C	228	LEU
1	C	239	MET
1	C	266	ARG
1	C	269	LEU
1	C	303	GLN

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Mol	Chain	Res	Type
1	C	306	GLN
1	C	322	TYR
1	C	338	ILE
1	C	339	VAL
1	D	100	VAL
1	D	239	MET
1	D	269	LEU
1	D	274	GLU
1	D	295	LEU
1	D	301	ASP
1	D	338	ILE
1	D	339	VAL
1	D	342	ARG
1	D	343	ASN
1	D	345	GLU
1	D	358	ASN
2	E	2	ASN
2	E	11	LYS
2	E	12	GLU
2	E	35	LEU
2	E	109	GLU
2	E	116	LEU
2	F	16	LEU
2	F	34	GLU
2	F	52	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	126	GLN
1	A	127	HIS
1	A	165	GLN
1	A	272	GLN
1	A	303	GLN
1	A	358	ASN
1	C	126	GLN
1	C	303	GLN
1	C	343	ASN
1	D	237	GLN
1	D	343	ASN

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5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	$\#|Z| > 2$
2	LA2	E	64	2	16,19,20	0.98	0	14,21,23	1.39	2 (14%)
2	LA2	F	64	2	16,19,20	0.95	0	14,21,23	2.03	6 (42%)

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	LA2	E	64	2	-	0/16/20/22	0/0/0/0
2	LA2	F	64	2	-	0/16/20/22	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	64	LA2	O1-C1-NZ	-2.90	117.18	122.94
2	E	64	LA2	O-C-CA	-2.79	118.23	125.49
2	F	64	LA2	O-C-CA	-2.19	119.78	125.49
2	F	64	LA2	C3-C4-C5	2.02	120.84	113.66
2	F	64	LA2	C4-C3-C2	2.38	122.00	113.29
2	E	64	LA2	C2-C1-NZ	2.76	121.25	116.46
2	F	64	LA2	C2-C1-NZ	3.74	122.96	116.46
2	F	64	LA2	C7-C6-C5	3.98	124.12	113.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	64	LA2	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	#$|Z| > 2$
3	C2F	A	401	-	25,35,35	1.62	5 (20%)	27,49,49	2.40	9 (33%)
3	C2F	B	401	-	25,35,35	1.72	4 (16%)	27,49,49	2.42	6 (22%)
3	C2F	C	401	-	25,35,35	1.40	2 (8%)	27,49,49	2.26	6 (22%)
4	PO4	C	501	-	4,4,4	0.53	0	6,6,6	0.29	0
3	C2F	D	401	-	25,35,35	1.24	2 (8%)	27,49,49	2.16	6 (22%)
4	PO4	D	501	-	4,4,4	0.24	0	6,6,6	0.33	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
3	C2F	A	401	-	-	0/16/35/35	0/3/3/3
3	C2F	B	401	-	-	0/16/35/35	0/3/3/3
3	C2F	C	401	-	-	0/16/35/35	0/3/3/3
4	PO4	C	501	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C2F	D	401	-	-	0/16/35/35	0/3/3/3
4	PO4	D	501	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	C2F	C6-N5	-2.94	1.44	1.47
3	A	401	C2F	C2-N1	-2.43	1.31	1.35
3	D	401	C2F	C6-N5	-2.12	1.45	1.47
3	A	401	C2F	C8A-N1	2.09	1.38	1.34
3	A	401	C2F	C7-N8	2.52	1.49	1.46
3	C	401	C2F	C7-N8	2.57	1.49	1.46
3	A	401	C2F	C2-N3	2.85	1.40	1.35
3	B	401	C2F	C8A-N1	3.01	1.40	1.34
3	B	401	C2F	O4-C4	3.90	1.34	1.24
3	D	401	C2F	O4-C4	4.24	1.34	1.24
3	C	401	C2F	O4-C4	4.55	1.35	1.24
3	B	401	C2F	C7-N8	5.54	1.53	1.46
3	A	401	C2F	O4-C4	5.75	1.38	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	C2F	C7-C6-N5	-10.00	97.70	108.79
3	D	401	C2F	C7-C6-N5	-7.75	100.19	108.79
3	A	401	C2F	C7-C6-N5	-6.82	101.22	108.79
3	A	401	C2F	C9-C6-N5	-5.89	98.58	110.90
3	C	401	C2F	C7-C6-N5	-5.43	102.77	108.79
3	C	401	C2F	C9-C6-N5	-4.23	102.06	110.90
3	D	401	C2F	C9-C6-N5	-3.64	103.29	110.90
3	C	401	C2F	C9-N10-C15	-3.28	113.20	121.46
3	A	401	C2F	C9-N10-C15	-2.83	114.32	121.46
3	B	401	C2F	N3-C2-N1	-2.78	120.97	125.53
3	A	401	C2F	C4A-C4-N3	-2.68	119.33	123.46
3	C	401	C2F	C4A-C4-N3	-2.43	119.73	123.46
3	D	401	C2F	N3-C2-N1	-2.30	121.76	125.53
3	C	401	C2F	C16-C17-C12	-2.13	118.30	120.76
3	A	401	C2F	N3-C2-N1	-2.08	122.12	125.53
3	A	401	C2F	C14-C13-C12	2.04	123.13	120.76
3	D	401	C2F	C4-N3-C2	2.12	118.88	115.94
3	B	401	C2F	C2-N1-C8A	2.22	119.52	114.54
3	D	401	C2F	C2-N1-C8A	2.91	121.08	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	C2F	C4-N3-C2	2.94	120.03	115.94
3	A	401	C2F	C4-N3-C2	3.02	120.12	115.94
3	A	401	C2F	NA2-C2-N3	3.07	122.28	117.20
3	B	401	C2F	C4-C4A-C8A	3.19	116.97	114.43
3	B	401	C2F	C6-C9-N10	3.25	119.79	111.54
3	D	401	C2F	C4-C4A-C8A	3.60	117.29	114.43
3	A	401	C2F	C4-C4A-C8A	4.09	117.69	114.43
3	C	401	C2F	C4-C4A-C8A	6.28	119.43	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	C2F	1	0
3	B	401	C2F	2	0
3	C	401	C2F	1	0
3	D	401	C2F	2	0
4	D	501	PO4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	363/364 (99%)	0.10	15 (4%)	41	42	10, 17, 39, 56	0
1	B	363/364 (99%)	0.05	12 (3%)	50	51	9, 18, 40, 52	0
1	C	363/364 (99%)	0.08	10 (2%)	56	57	11, 20, 43, 63	0
1	D	363/364 (99%)	0.10	13 (3%)	46	48	10, 20, 42, 68	0
2	E	127/129 (98%)	0.47	13 (10%)	9	9	18, 28, 62, 70	0
2	F	127/129 (98%)	0.52	9 (7%)	19	20	22, 36, 52, 65	0
All	All	1706/1714 (99%)	0.14	72 (4%)	40	41	9, 20, 47, 70	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	363	ALA	7.3
1	A	363	ALA	7.1
1	C	302	ALA	6.1
1	D	363	ALA	6.0
1	D	302	ALA	5.8
2	F	20	ALA	5.4
2	E	20	ALA	5.0
1	D	358	ASN	4.8
2	F	128	GLU	4.2
2	E	125	LEU	4.1
2	E	126	GLU	3.8
1	D	343	ASN	3.8
1	A	302	ALA	3.7
1	C	343	ASN	3.7
1	B	1[A]	ALA	3.6
1	A	46	PHE	3.5
1	C	340	GLN	3.5
1	A	343	ASN	3.4
2	F	126	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	5	ALA	3.3
1	D	342	ARG	3.3
1	C	362	VAL	3.3
1	D	303	GLN	3.2
2	E	128	GLU	3.2
1	B	343	ASN	3.2
1	B	274	GLU	3.1
1	B	302	ALA	3.1
1	A	362	VAL	3.0
1	C	342	ARG	3.0
1	A	360	LYS	2.9
2	F	1	SER	2.9
1	C	48	VAL	2.9
1	B	277	THR	2.9
1	A	358	ASN	2.9
1	A	342	ARG	2.8
1	C	275	HIS	2.8
2	E	124	LEU	2.8
1	A	359	GLY	2.8
2	F	5	ALA	2.7
2	E	119	THR	2.7
2	E	21	ASP	2.6
1	D	357	ARG	2.6
2	F	119	THR	2.5
1	D	275	HIS	2.5
2	E	109	GLU	2.5
1	B	46	PHE	2.4
1	B	21	HIS	2.4
1	D	209	ALA	2.4
1	B	338	ILE	2.4
1	A	188	TYR	2.3
1	D	362	VAL	2.3
1	C	322	TYR	2.3
2	E	115	LEU	2.2
1	A	144	ILE	2.2
2	E	1	SER	2.2
1	B	275	HIS	2.2
1	A	3	GLN	2.2
2	E	24	TYR	2.2
1	D	304	GLY	2.2
1	B	303	GLN	2.2
2	F	7	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	301	ASP	2.1
1	A	145	ALA	2.1
2	F	47	VAL	2.1
2	F	110	SER	2.1
1	B	187	GLY	2.1
2	E	110	SER	2.1
1	C	358	ASN	2.1
1	D	305	ASN	2.1
1	A	218	CYS	2.0
1	A	345	GLU	2.0
1	B	363	ALA	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, 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
2	LA2	F	64	20/21	0.92	0.13	-	23,41,44,48	0
2	LA2	E	64	20/21	0.92	0.15	-	20,33,47,52	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	C2F	A	401	33/33	0.88	0.19	1.15	9,21,44,47	0
3	C2F	C	401	33/33	0.89	0.21	1.13	11,26,43,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	C2F	D	401	33/33	0.93	0.16	0.95	11,25,48,50	0
3	C2F	B	401	33/33	0.93	0.15	0.64	10,19,42,45	0
4	PO4	C	501	5/5	0.97	0.09	-0.88	36,38,41,41	0
4	PO4	D	501	5/5	0.97	0.08	-1.66	37,38,39,43	0

6.5 Other polymers (i)

There are no such residues in this entry.