Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:42 AM GMT

PDB ID	:	2NU9
Title	:	C123aT Mutant of E. coli Succinyl-CoA Synthetase Orthorhombic Crystal Form
Authors	:	Fraser, M.E.
Deposited on	:	2006-11-08
Resolution	:	2.90 Å(reported)

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

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

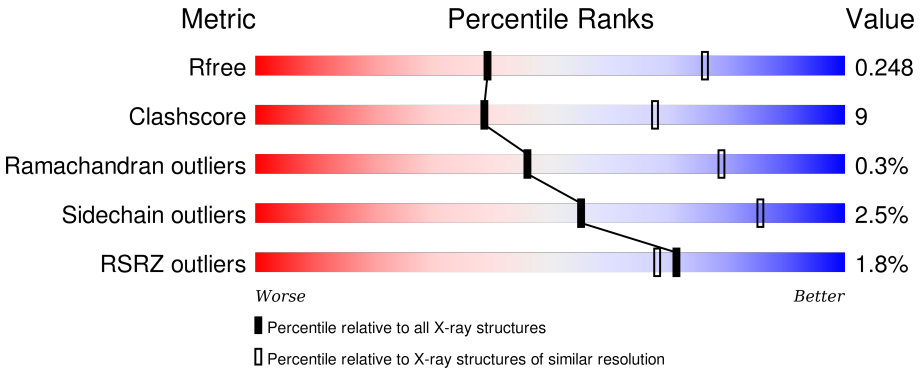
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	288	83% 15% ••
1	D	288	79% 19% ••
1	F	288	81% 18% ••
1	H	288	77% 21% ••
2	B	388	3% 79% 19% ••

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Mol	Chain	Length	Quality of chain
2	E	388	2% 78% 21%
2	G	388	3% 78% 20%
2	I	388	4% 76% 22%

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
3	SO4	I	389	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20040 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 Succinyl-CoA ligase [ADP-forming] subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	0
			2066	1308	345	402	1	10			
1	D	286	Total	C	N	O	P	S	0	0	0
			2066	1308	345	402	1	10			
1	F	286	Total	C	N	O	P	S	0	0	0
			2066	1308	345	402	1	10			
1	H	286	Total	C	N	O	P	S	0	0	0
			2066	1308	345	402	1	10			

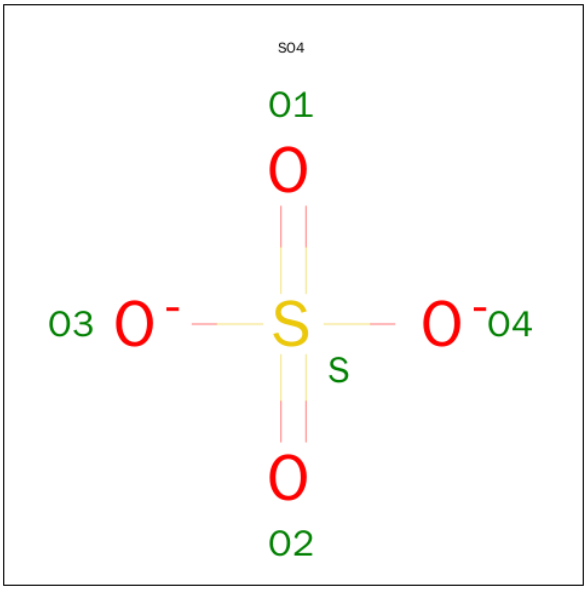
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	THR	CYS	ENGINEERED	UNP P0AGE9
A	246	NEP	HIS	MODIFIED RESIDUE	UNP P0AGE9
D	123	THR	CYS	ENGINEERED	UNP P0AGE9
D	246	NEP	HIS	MODIFIED RESIDUE	UNP P0AGE9
F	123	THR	CYS	ENGINEERED	UNP P0AGE9
F	246	NEP	HIS	MODIFIED RESIDUE	UNP P0AGE9
H	123	THR	CYS	ENGINEERED	UNP P0AGE9
H	246	NEP	HIS	MODIFIED RESIDUE	UNP P0AGE9

- Molecule 2 is a protein called Succinyl-CoA synthetase beta chain.

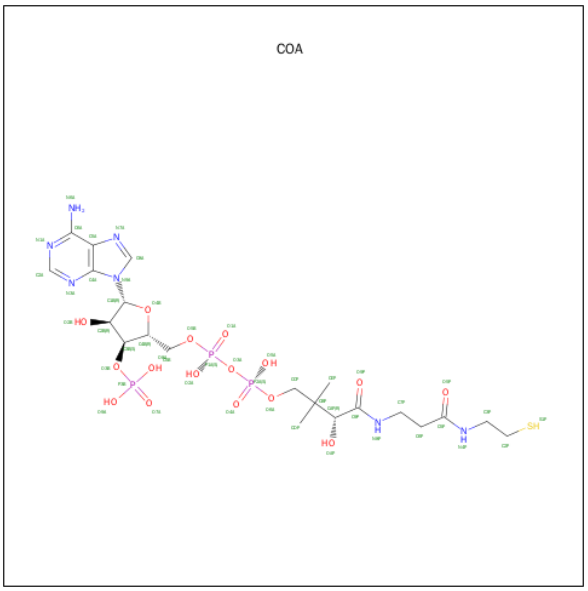
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2885	1823	505	544	13			
2	E	385	Total	C	N	O	S	0	0	0
			2885	1823	505	544	13			
2	G	385	Total	C	N	O	S	0	0	0
			2885	1823	505	544	13			
2	I	385	Total	C	N	O	S	0	0	0
			2885	1823	505	544	13			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 5 is water.

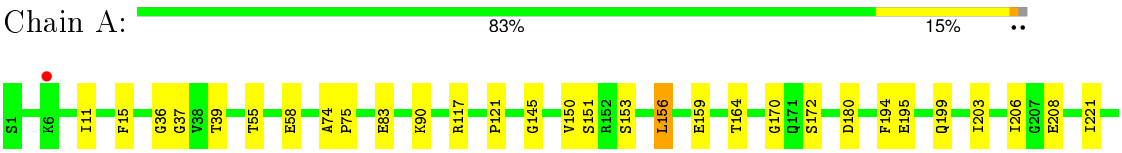
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		

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.

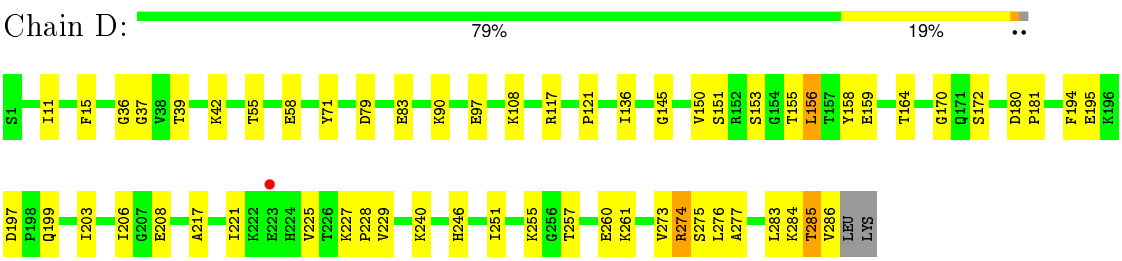
- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha

Chain A:



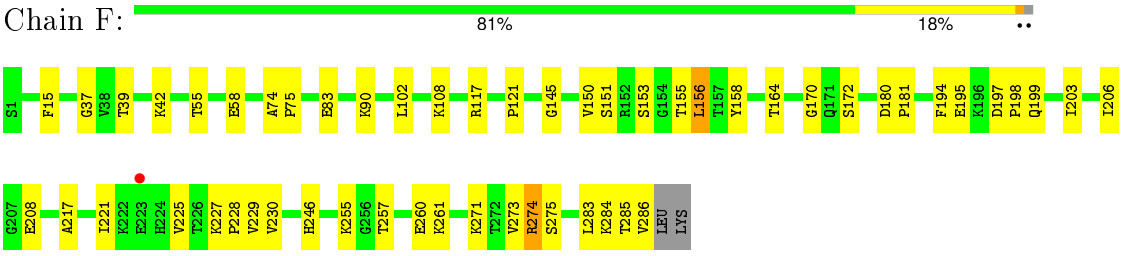
- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha

Chain D:



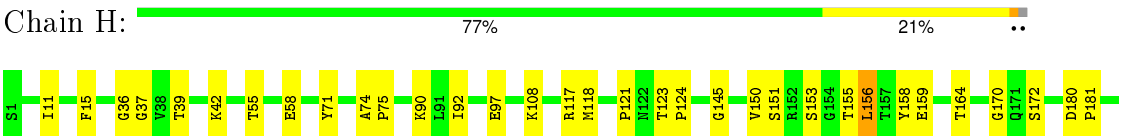
- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha

Chain F:

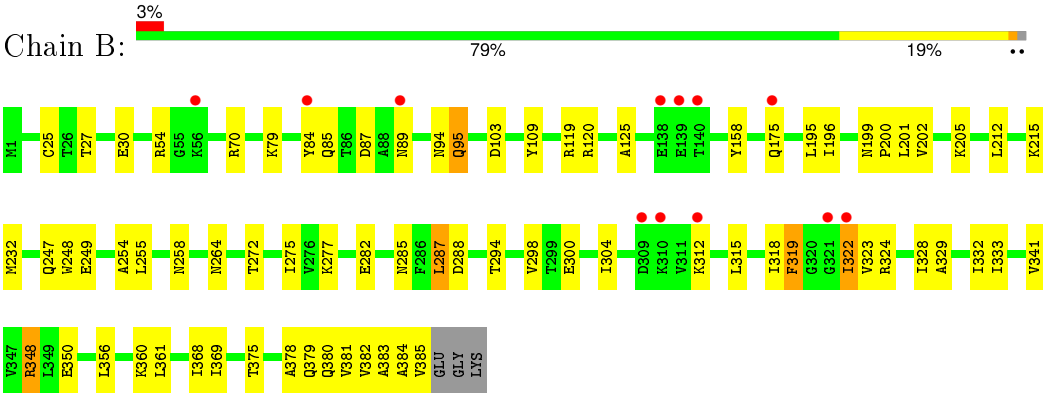


- Molecule 1: Succinyl-CoA ligase [ADP-forming] subunit alpha

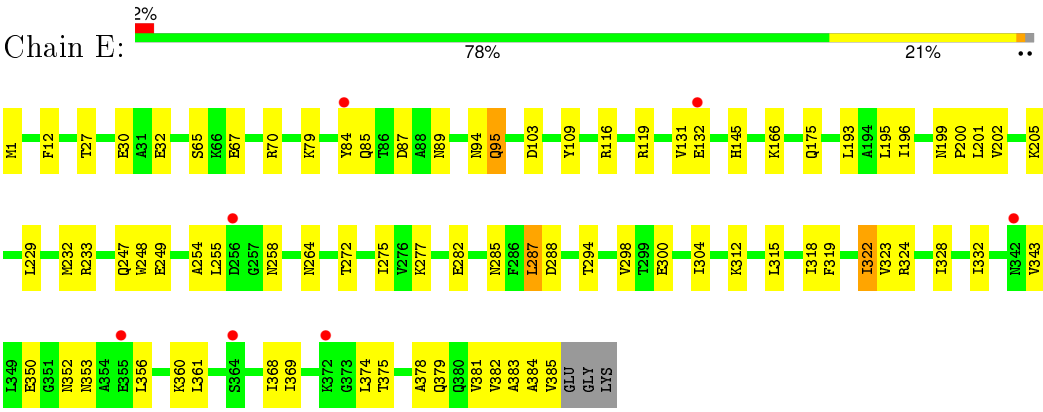
Chain H:



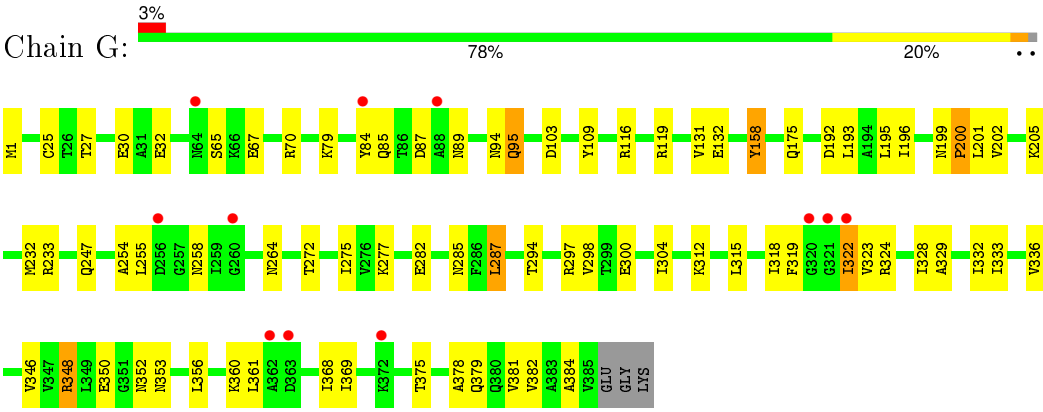
• Molecule 2: Succinyl-CoA synthetase beta chain



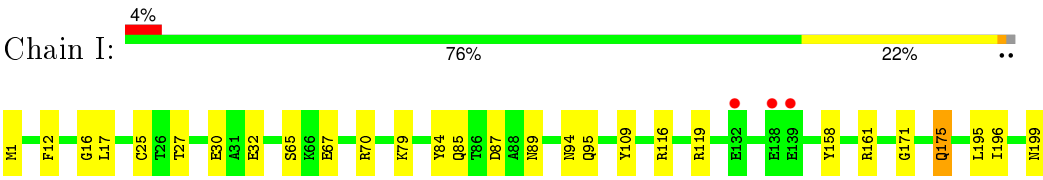
• Molecule 2: Succinyl-CoA synthetase beta chain

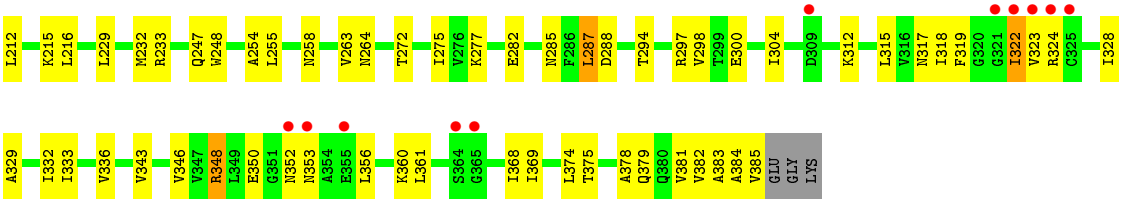


• Molecule 2: Succinyl-CoA synthetase beta chain



• Molecule 2: Succinyl-CoA synthetase beta chain




L212
K215
L216
L229
M232
R233
Q247
W248
A254
L255
N258
V263
N264
T272
I275
V276
K277
E282
N285
F286
L287
D288
T294
R297
V298
T299
E300
I304
D309
K312
L315
V316
N317
I318
F319
G320
G321
I322
V323
R324
C325
I328
A329
I332
I333
V336
V343
V346
V347
R348
L349
E350
G351
N352
N353
A354
E355
L356
K360
L361
S364
G385
I368
I369
L374
T375
A378
Q379
Q380
V381
V382
A383
A384
V385
GLU
GLY
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.53Å 154.90Å 240.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.11 – 2.90 20.10 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.11-2.90) 98.6 (20.10-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.251 0.228 , 0.248	Depositor DCC
R_{free} test set	4125 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 80943 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20040	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: COA, SO4, NEP

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	0.41	0/2084	0.63	0/2822
1	D	0.40	0/2084	0.64	0/2822
1	F	0.41	0/2084	0.64	0/2822
1	H	0.41	0/2084	0.64	0/2822
2	B	0.43	0/2927	0.62	1/3961 (0.0%)
2	E	0.42	0/2927	0.61	1/3961 (0.0%)
2	G	0.42	0/2927	0.61	1/3961 (0.0%)
2	I	0.42	0/2927	0.61	1/3961 (0.0%)
All	All	0.42	0/20044	0.62	4/27132 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	LEU	N-CA-C	-5.53	96.08	111.00
2	G	201	LEU	N-CA-C	-5.22	96.90	111.00
2	I	201	LEU	N-CA-C	-5.07	97.32	111.00
2	E	201	LEU	N-CA-C	-5.01	97.47	111.00

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	2066	0	2118	29	0
1	D	2066	0	2118	42	0
1	F	2066	0	2118	36	0
1	H	2066	0	2118	42	0
2	B	2885	0	2941	61	0
2	E	2885	0	2941	60	0
2	G	2885	0	2941	58	0
2	I	2885	0	2941	64	0
3	B	10	0	0	1	0
3	E	10	0	0	0	0
3	G	10	0	0	0	0
3	I	10	0	0	0	0
4	A	48	0	32	1	0
4	D	48	0	32	5	0
4	F	48	0	32	0	0
4	H	48	0	32	3	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
All	All	20040	0	20364	365	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 9.

All (365) 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)
2:I:322:ILE:HD13	2:I:322:ILE:H	1.29	0.97
2:E:322:ILE:HD13	2:E:322:ILE:H	1.26	0.97
2:G:322:ILE:H	2:G:322:ILE:HD13	1.27	0.96
2:B:322:ILE:H	2:B:322:ILE:HD13	1.31	0.94
2:E:315:LEU:HB2	2:E:381:VAL:HG11	1.56	0.87
2:G:94:ASN:HD22	2:I:247:GLN:HE22	1.23	0.84
2:I:315:LEU:HB2	2:I:381:VAL:HG11	1.59	0.84
2:G:315:LEU:HB2	2:G:381:VAL:HG11	1.61	0.82
2:B:315:LEU:HB2	2:B:381:VAL:HG11	1.59	0.82
2:G:247:GLN:HE22	2:I:94:ASN:HD22	1.24	0.82
2:B:158:TYR:CD1	1:F:83:GLU:HG3	2.18	0.79
1:F:195:GLU:OE1	1:F:225:VAL:HA	1.93	0.68
2:B:94:ASN:HD22	2:E:247:GLN:HE22	1.42	0.68
1:H:195:GLU:OE1	1:H:225:VAL:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:322:ILE:HD13	2:E:322:ILE:N	2.06	0.66
1:A:195:GLU:OE1	1:A:225:VAL:HA	1.95	0.66
2:G:322:ILE:HD13	2:G:322:ILE:N	2.07	0.66
1:D:285:THR:O	1:D:285:THR:HG22	1.96	0.66
1:D:195:GLU:OE1	1:D:225:VAL:HA	1.96	0.65
1:D:83:GLU:HG3	2:I:158:TYR:CD1	2.31	0.65
1:A:285:THR:HG22	1:A:285:THR:O	1.98	0.64
2:E:229:LEU:HD23	2:E:232:MET:HE3	1.80	0.64
1:F:285:THR:O	1:F:285:THR:HG22	1.99	0.63
2:I:322:ILE:N	2:I:322:ILE:HD13	2.09	0.62
2:B:369:ILE:HD12	2:B:369:ILE:N	2.15	0.62
2:B:312:LYS:O	2:B:343:VAL:HB	2.00	0.62
1:H:285:THR:O	1:H:285:THR:HG22	1.99	0.62
1:A:273:VAL:HG12	1:A:275:SER:H	1.65	0.62
2:B:70:ARG:NH2	2:E:249:GLU:OE1	2.34	0.61
2:G:312:LYS:O	2:G:343:VAL:HB	2.00	0.61
2:B:247:GLN:HE22	2:E:94:ASN:HD22	1.48	0.61
2:E:277:LYS:HE2	2:E:282:GLU:OE2	2.03	0.59
2:B:277:LYS:HE2	2:B:282:GLU:OE2	2.03	0.59
2:E:79:LYS:HD2	2:E:79:LYS:N	2.19	0.58
1:F:273:VAL:HG12	1:F:275:SER:H	1.67	0.58
1:D:273:VAL:HG12	1:D:275:SER:H	1.68	0.58
2:B:322:ILE:HD13	2:B:322:ILE:N	2.12	0.58
2:I:322:ILE:CD1	2:I:322:ILE:H	2.09	0.58
2:G:322:ILE:CD1	2:G:322:ILE:H	2.08	0.58
2:B:254:ALA:C	2:B:255:LEU:HD12	2.24	0.57
2:E:312:LYS:O	2:E:343:VAL:HB	2.03	0.57
1:H:273:VAL:HG12	1:H:275:SER:H	1.68	0.57
2:B:84:TYR:CE1	2:B:85:GLN:HG3	2.39	0.57
2:I:369:ILE:HD12	2:I:369:ILE:N	2.20	0.57
2:E:356:LEU:O	2:E:360:LYS:HG3	2.05	0.57
2:G:277:LYS:HE2	2:G:282:GLU:OE2	2.05	0.56
2:G:84:TYR:CE1	2:G:85:GLN:HG3	2.40	0.56
2:I:312:LYS:O	2:I:343:VAL:HB	2.04	0.56
2:I:254:ALA:C	2:I:255:LEU:HD12	2.24	0.56
2:E:254:ALA:C	2:E:255:LEU:HD12	2.26	0.56
2:B:54:ARG:HB2	3:B:389:SO4:O3	2.06	0.56
2:G:254:ALA:C	2:G:255:LEU:HD12	2.26	0.56
2:G:356:LEU:O	2:G:360:LYS:HG3	2.06	0.56
2:I:356:LEU:O	2:I:360:LYS:HG3	2.05	0.56
2:I:277:LYS:HE2	2:I:282:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:THR:OG1	1:A:260:GLU:HB2	2.07	0.55
2:G:369:ILE:HD12	2:G:369:ILE:N	2.21	0.55
2:E:369:ILE:HD12	2:E:369:ILE:N	2.22	0.55
2:I:84:TYR:CE1	2:I:85:GLN:HG3	2.42	0.55
1:D:97:GLU:HB3	4:D:301:COA:H71	1.88	0.54
2:B:356:LEU:O	2:B:360:LYS:HG3	2.06	0.54
2:I:328:ILE:O	2:I:332:ILE:HG13	2.07	0.54
2:B:229:LEU:HD23	2:B:232:MET:HE3	1.90	0.54
2:E:84:TYR:CE1	2:E:85:GLN:HG3	2.43	0.54
1:H:150:VAL:HG22	1:H:194:PHE:HE2	1.73	0.54
2:B:249:GLU:OE1	2:E:70:ARG:NH2	2.41	0.54
2:B:79:LYS:N	2:B:79:LYS:HD2	2.23	0.54
2:E:348:ARG:NH1	2:E:350:GLU:HB2	2.23	0.53
1:F:55:THR:OG1	1:F:58:GLU:HG3	2.08	0.53
1:D:150:VAL:HG22	1:D:194:PHE:HE2	1.73	0.53
1:H:55:THR:OG1	1:H:58:GLU:HG3	2.09	0.53
1:D:257:THR:OG1	1:D:260:GLU:HB2	2.08	0.53
2:B:87:ASP:OD1	2:B:89:ASN:N	2.42	0.53
2:G:79:LYS:N	2:G:79:LYS:HD2	2.24	0.53
2:B:328:ILE:O	2:B:332:ILE:HG13	2.10	0.52
1:H:257:THR:OG1	1:H:260:GLU:HB2	2.10	0.52
2:G:229:LEU:HA	2:G:232:MET:HE2	1.92	0.52
2:I:79:LYS:HD2	2:I:79:LYS:N	2.24	0.52
2:I:202:VAL:HG21	2:I:212:LEU:HD22	1.92	0.52
2:E:322:ILE:H	2:E:322:ILE:CD1	2.07	0.51
2:B:369:ILE:HD12	2:B:369:ILE:H	1.74	0.51
1:H:172:SER:HA	1:H:199:GLN:NE2	2.25	0.51
1:A:150:VAL:HG22	1:A:194:PHE:HE2	1.75	0.51
2:B:375:THR:O	2:B:379:GLN:HG3	2.10	0.51
1:F:257:THR:OG1	1:F:260:GLU:HB2	2.10	0.51
1:F:150:VAL:HG22	1:F:194:PHE:HE2	1.76	0.51
1:D:55:THR:OG1	1:D:58:GLU:HG3	2.11	0.51
2:G:369:ILE:HD12	2:G:369:ILE:H	1.76	0.50
2:I:229:LEU:HA	2:I:232:MET:HE2	1.92	0.50
2:G:229:LEU:HD23	2:G:232:MET:HE3	1.93	0.50
2:B:287:LEU:C	2:B:287:LEU:HD12	2.31	0.50
2:E:328:ILE:O	2:E:332:ILE:HG13	2.11	0.50
1:H:276:LEU:HD11	2:I:374:LEU:CD2	2.41	0.50
1:D:153:SER:HB3	1:D:246:NEP:HE1	1.92	0.50
1:A:55:THR:OG1	1:A:58:GLU:HG3	2.10	0.50
1:A:156:LEU:HD13	1:A:206:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:328:ILE:O	2:G:332:ILE:HG13	2.11	0.50
1:A:172:SER:HA	1:A:199:GLN:NE2	2.27	0.50
2:B:348:ARG:NH1	2:B:350:GLU:HB2	2.27	0.50
2:E:287:LEU:C	2:E:287:LEU:HD12	2.31	0.50
2:E:369:ILE:HD12	2:E:369:ILE:H	1.77	0.50
2:G:202:VAL:HG21	2:G:212:LEU:HD22	1.94	0.50
1:A:153:SER:HB3	1:A:246:NEP:HE1	1.93	0.50
2:I:375:THR:O	2:I:379:GLN:HG3	2.12	0.50
1:D:172:SER:HA	1:D:199:GLN:NE2	2.25	0.50
1:A:164:THR:HG22	1:A:283:LEU:CD1	2.42	0.50
2:I:348:ARG:NH1	2:I:350:GLU:HB2	2.26	0.49
2:I:369:ILE:H	2:I:369:ILE:HD12	1.76	0.49
2:E:375:THR:O	2:E:379:GLN:HG3	2.13	0.49
2:G:287:LEU:C	2:G:287:LEU:HD12	2.33	0.49
2:B:202:VAL:HG21	2:B:212:LEU:HD22	1.92	0.49
1:D:108:LYS:HG2	2:E:119:ARG:HD2	1.95	0.49
2:B:255:LEU:HD13	2:B:285:ASN:HA	1.94	0.49
2:G:348:ARG:NH1	2:G:350:GLU:HB2	2.26	0.49
1:H:153:SER:HB3	1:H:246:NEP:HE1	1.94	0.49
2:E:87:ASP:OD1	2:E:89:ASN:N	2.46	0.49
1:H:164:THR:HG22	1:H:283:LEU:CD1	2.42	0.49
1:F:208:GLU:O	1:F:261:LYS:HE3	2.13	0.49
2:I:294:THR:O	2:I:298:VAL:HG23	2.12	0.49
2:B:109:TYR:C	2:B:109:TYR:CD1	2.85	0.49
1:D:156:LEU:HD13	1:D:206:ILE:HG21	1.95	0.49
2:B:229:LEU:HA	2:B:232:MET:HE2	1.95	0.48
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.94	0.48
2:I:229:LEU:HD23	2:I:232:MET:CE	2.43	0.48
2:B:229:LEU:HD23	2:B:232:MET:CE	2.43	0.48
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.78	0.48
1:F:172:SER:HA	1:F:199:GLN:NE2	2.28	0.48
2:G:375:THR:O	2:G:379:GLN:HG3	2.13	0.48
2:I:272:THR:O	2:I:275:ILE:HG22	2.14	0.48
2:B:300:GLU:O	2:B:304:ILE:HG13	2.14	0.48
2:I:346:VAL:HB	2:I:381:VAL:CG1	2.43	0.48
2:I:287:LEU:C	2:I:287:LEU:HD12	2.33	0.48
2:G:87:ASP:OD1	2:G:89:ASN:N	2.44	0.48
2:G:109:TYR:CD1	2:G:109:TYR:C	2.87	0.48
1:F:164:THR:HG22	1:F:283:LEU:CD1	2.44	0.48
1:D:164:THR:HG22	1:D:283:LEU:CD1	2.43	0.48
2:G:255:LEU:HD13	2:G:285:ASN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:TYR:C	4:D:301:COA:H142	2.34	0.47
1:F:153:SER:HB3	1:F:246:NEP:HE1	1.95	0.47
2:E:109:TYR:C	2:E:109:TYR:CD1	2.88	0.47
1:F:156:LEU:HD13	1:F:206:ILE:HG21	1.96	0.47
1:D:136:ILE:HD11	4:D:301:COA:H21	1.97	0.47
2:E:300:GLU:O	2:E:304:ILE:HG13	2.13	0.47
2:I:109:TYR:C	2:I:109:TYR:CD1	2.86	0.47
1:D:284:LYS:C	1:D:286:VAL:H	2.17	0.47
2:B:264:ASN:OD1	2:B:318:ILE:HA	2.14	0.47
2:G:27:THR:OG1	2:G:30:GLU:HG3	2.14	0.47
2:I:361:LEU:HD22	2:I:368:ILE:HG21	1.97	0.47
1:H:274:ARG:HH11	1:H:274:ARG:HG3	1.80	0.47
2:B:322:ILE:CD1	2:B:322:ILE:H	2.12	0.47
2:I:332:ILE:O	2:I:336:VAL:HG23	2.14	0.47
1:A:156:LEU:HD13	1:A:206:ILE:CG2	2.44	0.47
1:H:284:LYS:C	1:H:286:VAL:H	2.18	0.47
1:F:121:PRO:HG2	1:F:180:ASP:OD2	2.14	0.47
2:B:294:THR:O	2:B:298:VAL:HG23	2.15	0.47
1:D:15:PHE:CG	1:D:37:GLY:HA3	2.49	0.47
2:B:215:LYS:O	2:B:216:LEU:HD23	2.15	0.47
1:D:156:LEU:HD13	1:D:206:ILE:CG2	2.44	0.47
1:F:181:PRO:CA	2:G:116:ARG:HD3	2.44	0.47
1:D:203:ILE:HB	1:D:229:VAL:HG22	1.96	0.47
1:H:159:GLU:OE2	2:I:348:ARG:NH2	2.47	0.47
2:G:229:LEU:HD23	2:G:232:MET:CE	2.45	0.47
1:A:284:LYS:C	1:A:286:VAL:H	2.19	0.47
2:B:272:THR:O	2:B:275:ILE:HG22	2.15	0.47
2:G:378:ALA:O	2:G:382:VAL:HG23	2.14	0.46
1:F:108:LYS:HG2	2:G:119:ARG:HD2	1.96	0.46
1:A:83:GLU:HG3	2:G:158:TYR:CD1	2.50	0.46
2:E:229:LEU:HD23	2:E:232:MET:CE	2.44	0.46
1:D:159:GLU:OE2	2:E:348:ARG:NH2	2.48	0.46
2:G:346:VAL:HB	2:G:381:VAL:CG1	2.46	0.46
2:G:300:GLU:O	2:G:304:ILE:HG13	2.15	0.46
1:H:156:LEU:HD13	1:H:206:ILE:HG21	1.98	0.46
1:D:181:PRO:CA	2:E:116:ARG:HD3	2.45	0.46
2:E:346:VAL:HB	2:E:381:VAL:CG1	2.46	0.46
1:F:284:LYS:C	1:F:286:VAL:H	2.18	0.46
2:I:300:GLU:O	2:I:304:ILE:HG13	2.15	0.46
1:H:156:LEU:HD13	1:H:206:ILE:CG2	2.46	0.46
1:D:121:PRO:HG2	1:D:180:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:HG23	4:A:300:COA:O2B	2.16	0.46
2:E:202:VAL:HG21	2:E:212:LEU:HD22	1.98	0.46
2:E:323:VAL:HG12	2:E:324:ARG:N	2.31	0.46
1:A:159:GLU:OE2	2:B:348:ARG:NH2	2.49	0.46
1:F:156:LEU:HD13	1:F:206:ILE:CG2	2.45	0.46
1:D:208:GLU:O	1:D:261:LYS:HE3	2.16	0.46
1:D:71:TYR:O	4:D:301:COA:H142	2.16	0.46
1:H:276:LEU:HD11	2:I:374:LEU:HD23	1.97	0.46
2:B:84:TYR:CD1	2:B:85:GLN:HG3	2.51	0.46
1:H:108:LYS:HG2	2:I:119:ARG:HD2	1.97	0.45
2:E:199:ASN:HA	2:E:200:PRO:HA	1.71	0.45
2:I:248:TRP:CD1	2:I:300:GLU:HG3	2.51	0.45
2:B:346:VAL:HB	2:B:381:VAL:CG1	2.46	0.45
1:D:217:ALA:O	1:D:221:ILE:HG13	2.16	0.45
2:I:229:LEU:HD23	2:I:232:MET:HE3	1.97	0.45
1:F:15:PHE:CG	1:F:37:GLY:HA3	2.50	0.45
1:A:208:GLU:O	1:A:261:LYS:HE3	2.16	0.45
1:F:203:ILE:HB	1:F:229:VAL:HG22	1.98	0.45
2:E:27:THR:OG1	2:E:30:GLU:HG3	2.17	0.45
2:I:255:LEU:HD13	2:I:285:ASN:HA	1.98	0.45
1:H:39:THR:HG23	4:H:401:COA:O2B	2.16	0.45
2:G:294:THR:O	2:G:298:VAL:HG23	2.16	0.45
2:I:27:THR:OG1	2:I:30:GLU:HG3	2.16	0.45
2:B:158:TYR:CG	1:F:83:GLU:HG3	2.51	0.45
2:I:323:VAL:HG12	2:I:324:ARG:N	2.31	0.45
2:B:323:VAL:HG12	2:B:324:ARG:N	2.31	0.45
1:F:151:SER:HB2	1:F:206:ILE:HB	1.99	0.45
1:F:274:ARG:HH11	1:F:274:ARG:HG3	1.81	0.45
1:D:79:ASP:OD2	2:I:161:ARG:NH2	2.48	0.45
1:D:15:PHE:CD2	1:D:37:GLY:HA3	2.52	0.45
2:I:171:GLY:O	2:I:175:GLN:NE2	2.50	0.45
1:D:145:GLY:HA3	1:D:170:GLY:HA3	1.99	0.45
2:G:84:TYR:CD1	2:G:85:GLN:HG3	2.52	0.45
1:A:15:PHE:CG	1:A:37:GLY:HA3	2.52	0.45
1:H:208:GLU:O	1:H:261:LYS:HE3	2.16	0.45
1:D:274:ARG:HG3	1:D:274:ARG:HH11	1.81	0.45
1:H:121:PRO:HG2	1:H:180:ASP:OD2	2.17	0.45
1:H:181:PRO:CA	2:I:116:ARG:HD3	2.47	0.44
1:F:15:PHE:CD2	1:F:37:GLY:HA3	2.52	0.44
1:F:74:ALA:HB3	1:F:75:PRO:HD3	1.98	0.44
2:E:12:PHE:CZ	2:E:216:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LEU:HD22	2:B:368:ILE:HG21	1.98	0.44
1:A:203:ILE:HB	1:A:229:VAL:HG22	2.00	0.44
2:E:378:ALA:O	2:E:382:VAL:HG23	2.16	0.44
1:H:151:SER:HB2	1:H:206:ILE:HB	1.99	0.44
2:G:199:ASN:HA	2:G:200:PRO:HA	1.69	0.44
2:B:195:LEU:HG	2:B:196:ILE:N	2.32	0.44
1:H:221:ILE:HG23	1:H:225:VAL:HB	2.00	0.44
2:E:229:LEU:HA	2:E:232:MET:HE2	2.00	0.44
2:I:378:ALA:O	2:I:382:VAL:HG23	2.17	0.44
1:F:181:PRO:HA	2:G:116:ARG:HD3	1.99	0.44
1:H:97:GLU:HB3	4:H:401:COA:H71	1.99	0.44
2:B:378:ALA:O	2:B:382:VAL:HG23	2.17	0.44
1:D:221:ILE:HG23	1:D:225:VAL:HB	2.00	0.44
2:B:199:ASN:HA	2:B:200:PRO:HA	1.71	0.44
1:H:197:ASP:O	1:H:227:LYS:NZ	2.51	0.44
2:E:272:THR:O	2:E:275:ILE:HG22	2.18	0.43
1:H:39:THR:HG21	1:H:42:LYS:HD2	2.00	0.43
2:E:95:GLN:HB2	2:E:95:GLN:HE21	1.40	0.43
2:G:65:SER:HB2	2:G:67:GLU:OE1	2.19	0.43
2:B:95:GLN:HB2	2:B:95:GLN:HE21	1.42	0.43
1:H:74:ALA:HB3	1:H:75:PRO:HD3	1.99	0.43
2:B:103:ASP:HB3	2:B:205:LYS:HG3	1.99	0.43
2:E:294:THR:O	2:E:298:VAL:HG23	2.17	0.43
2:G:272:THR:O	2:G:275:ILE:HG22	2.18	0.43
2:G:32:GLU:OE1	2:G:70:ARG:HD2	2.17	0.43
2:G:131:VAL:HG12	2:G:132:GLU:N	2.34	0.43
2:G:341:VAL:HG12	2:G:343:VAL:H	1.84	0.43
2:I:84:TYR:CD1	2:I:85:GLN:HG3	2.54	0.43
1:D:136:ILE:CD1	4:D:301:COA:H21	2.49	0.43
2:I:119:ARG:HH11	2:I:119:ARG:HG3	1.83	0.43
2:E:193:LEU:HD12	2:E:196:ILE:HD11	1.99	0.43
1:A:121:PRO:HG2	1:A:180:ASP:OD2	2.19	0.43
2:G:323:VAL:HG12	2:G:324:ARG:N	2.34	0.43
1:D:197:ASP:O	1:D:227:LYS:NZ	2.52	0.43
2:G:361:LEU:HD22	2:G:368:ILE:HG21	2.00	0.43
1:F:102:LEU:HD12	2:G:192:ASP:HA	2.01	0.43
2:G:1:MET:SD	2:G:233:ARG:HB2	2.59	0.43
1:A:15:PHE:CD2	1:A:37:GLY:HA3	2.53	0.43
2:E:264:ASN:OD1	2:E:318:ILE:HA	2.19	0.43
1:F:39:THR:HG21	1:F:42:LYS:HD2	2.00	0.42
1:A:145:GLY:HA3	1:A:170:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:PHE:CG	1:H:37:GLY:HA3	2.53	0.42
1:H:145:GLY:HA3	1:H:170:GLY:HA3	2.01	0.42
1:A:151:SER:HB2	1:A:206:ILE:HB	2.01	0.42
2:E:287:LEU:HD12	2:E:288:ASP:N	2.33	0.42
1:D:151:SER:HB2	1:D:206:ILE:HB	2.01	0.42
1:H:228:PRO:CB	1:H:286:VAL:HG11	2.50	0.42
1:H:228:PRO:HB3	1:H:286:VAL:HG11	2.01	0.42
1:A:11:ILE:HA	1:A:36:GLY:O	2.19	0.42
1:D:240:LYS:HA	1:D:251:ILE:HB	2.01	0.42
2:I:297:ARG:HG3	2:I:297:ARG:HH11	1.84	0.42
2:G:264:ASN:OD1	2:G:318:ILE:HA	2.18	0.42
2:I:87:ASP:OD1	2:I:89:ASN:N	2.48	0.42
1:D:285:THR:CG2	1:D:285:THR:O	2.65	0.42
2:I:254:ALA:O	2:I:255:LEU:HD12	2.19	0.42
1:F:228:PRO:CB	1:F:286:VAL:HG11	2.49	0.42
1:F:230:VAL:HA	1:F:271:LYS:O	2.19	0.42
2:E:1:MET:SD	2:E:233:ARG:HB2	2.59	0.42
1:H:230:VAL:HA	1:H:271:LYS:O	2.20	0.42
1:F:197:ASP:HA	1:F:198:PRO:HD2	1.94	0.42
1:F:217:ALA:O	1:F:221:ILE:HG13	2.19	0.42
2:E:84:TYR:CD1	2:E:85:GLN:HG3	2.55	0.42
2:B:248:TRP:CD1	2:B:300:GLU:HG3	2.54	0.42
2:B:381:VAL:HG23	2:B:382:VAL:N	2.34	0.42
2:B:287:LEU:HD12	2:B:288:ASP:N	2.35	0.42
1:H:11:ILE:HA	1:H:36:GLY:O	2.20	0.42
2:I:264:ASN:OD1	2:I:318:ILE:HA	2.19	0.42
2:G:381:VAL:HG23	2:G:382:VAL:N	2.35	0.42
2:E:383:ALA:O	2:E:385:VAL:N	2.53	0.42
2:I:329:ALA:O	2:I:333:ILE:HG13	2.19	0.42
1:F:145:GLY:HA3	1:F:170:GLY:HA3	2.01	0.42
2:I:346:VAL:HB	2:I:381:VAL:HG13	2.02	0.42
1:H:217:ALA:O	1:H:221:ILE:HG13	2.20	0.42
1:A:221:ILE:HG23	1:A:225:VAL:HB	2.01	0.42
1:H:15:PHE:CD2	1:H:37:GLY:HA3	2.55	0.42
2:I:32:GLU:OE1	2:I:70:ARG:HD2	2.20	0.42
2:B:25:CYS:HB3	2:B:30:GLU:HB2	2.02	0.42
1:D:276:LEU:HD11	2:E:374:LEU:HD23	2.02	0.42
2:G:352:ASN:O	2:G:353:ASN:HB2	2.20	0.41
2:G:193:LEU:HD12	2:G:196:ILE:HD11	2.01	0.41
2:I:12:PHE:CZ	2:I:216:LEU:HD21	2.54	0.41
2:B:27:THR:OG1	2:B:30:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:THR:HA	1:H:158:TYR:CD2	2.55	0.41
2:E:131:VAL:HG12	2:E:132:GLU:N	2.35	0.41
2:B:380:GLN:O	2:B:383:ALA:HB3	2.19	0.41
1:D:11:ILE:HA	1:D:36:GLY:O	2.20	0.41
2:G:94:ASN:HD22	2:I:247:GLN:NE2	2.04	0.41
2:E:119:ARG:HG3	2:E:119:ARG:HH11	1.85	0.41
1:D:228:PRO:HB3	1:D:286:VAL:HG11	2.01	0.41
2:I:352:ASN:O	2:I:353:ASN:HB2	2.20	0.41
2:E:361:LEU:HD22	2:E:368:ILE:HG21	2.02	0.41
2:I:195:LEU:HG	2:I:196:ILE:N	2.34	0.41
2:E:381:VAL:HG23	2:E:382:VAL:N	2.36	0.41
2:G:322:ILE:CD1	2:G:322:ILE:N	2.76	0.41
1:A:275:SER:C	1:A:277:ALA:N	2.73	0.41
2:G:332:ILE:O	2:G:336:VAL:HG23	2.20	0.41
1:F:197:ASP:O	1:F:227:LYS:NZ	2.53	0.41
1:H:275:SER:HB3	1:H:278:ASP:OD2	2.21	0.41
2:B:383:ALA:O	2:B:385:VAL:N	2.53	0.41
2:B:119:ARG:HG3	2:B:119:ARG:HH11	1.86	0.41
2:G:297:ARG:HH11	2:G:297:ARG:HG3	1.85	0.41
1:D:39:THR:HG21	1:D:42:LYS:HD2	2.03	0.41
2:G:329:ALA:O	2:G:333:ILE:HG13	2.21	0.41
2:I:287:LEU:HD12	2:I:288:ASP:N	2.36	0.41
2:E:248:TRP:CD1	2:E:300:GLU:HG3	2.56	0.41
1:F:228:PRO:HB3	1:F:286:VAL:HG11	2.01	0.41
1:H:71:TYR:C	4:H:401:COA:H142	2.41	0.41
2:I:25:CYS:HB3	2:I:30:GLU:HB2	2.02	0.41
2:I:16:GLY:C	2:I:17:LEU:HD23	2.41	0.41
1:F:155:THR:HA	1:F:158:TYR:CD2	2.55	0.41
1:H:92:ILE:O	1:H:118:MET:HA	2.21	0.41
2:B:329:ALA:O	2:B:333:ILE:HG13	2.20	0.41
1:A:285:THR:O	1:A:285:THR:CG2	2.67	0.41
1:D:275:SER:C	1:D:277:ALA:N	2.73	0.41
1:H:275:SER:C	1:H:277:ALA:N	2.75	0.41
2:E:255:LEU:HD13	2:E:285:ASN:HA	2.01	0.41
2:B:323:VAL:HG12	2:B:324:ARG:H	1.86	0.41
2:I:1:MET:SD	2:I:233:ARG:HB2	2.60	0.41
2:E:65:SER:HB2	2:E:67:GLU:OE1	2.20	0.41
1:H:203:ILE:HB	1:H:229:VAL:HG22	2.02	0.41
2:I:263:VAL:HG22	2:I:317:ASN:HB3	2.03	0.41
2:B:120:ARG:HH11	2:B:120:ARG:HG2	1.85	0.41
2:B:319:PHE:C	2:B:319:PHE:CD1	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:65:SER:HB2	2:I:67:GLU:OE1	2.20	0.41
2:B:70:ARG:HH22	2:E:249:GLU:CD	2.24	0.40
2:E:32:GLU:OE1	2:E:70:ARG:HD2	2.21	0.40
1:A:228:PRO:HB3	1:A:286:VAL:HG11	2.04	0.40
2:E:323:VAL:HG12	2:E:324:ARG:H	1.86	0.40
2:E:352:ASN:O	2:E:353:ASN:HB2	2.21	0.40
2:E:195:LEU:HG	2:E:196:ILE:N	2.35	0.40
2:I:215:LYS:O	2:I:216:LEU:HD23	2.22	0.40
2:E:103:ASP:HB3	2:E:205:LYS:HG3	2.02	0.40
1:H:123:THR:OG1	1:H:124:PRO:HD2	2.21	0.40
1:F:221:ILE:HG23	1:F:225:VAL:HB	2.04	0.40
2:B:341:VAL:HG12	2:B:343:VAL:H	1.87	0.40
2:B:212:LEU:HD12	2:B:212:LEU:HA	1.88	0.40
2:G:103:ASP:HB3	2:G:205:LYS:HG3	2.04	0.40
2:G:95:GLN:HE21	2:G:95:GLN:HB2	1.39	0.40
2:B:109:TYR:O	2:B:125:ALA:HA	2.22	0.40
2:G:25:CYS:HB3	2:G:30:GLU:HB2	2.04	0.40
2:I:383:ALA:O	2:I:385:VAL:N	2.54	0.40
1:D:228:PRO:CB	1:D:286:VAL:HG11	2.51	0.40
2:G:195:LEU:HG	2:G:196:ILE:N	2.35	0.40
1:D:155:THR:HA	1:D:158:TYR:CD2	2.56	0.40
2:E:145:HIS:ND1	2:E:166:LYS:HD3	2.37	0.40
2:I:199:ASN:HA	2:I:200:PRO:HA	1.71	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	283/288 (98%)	272 (96%)	10 (4%)	1 (0%)	39	74
1	D	283/288 (98%)	271 (96%)	11 (4%)	1 (0%)	39	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	283/288 (98%)	271 (96%)	12 (4%)	0	100	100
1	H	283/288 (98%)	271 (96%)	11 (4%)	1 (0%)	39	74
2	B	383/388 (99%)	373 (97%)	9 (2%)	1 (0%)	46	79
2	E	383/388 (99%)	373 (97%)	9 (2%)	1 (0%)	46	79
2	G	383/388 (99%)	372 (97%)	10 (3%)	1 (0%)	46	79
2	I	383/388 (99%)	373 (97%)	9 (2%)	1 (0%)	46	79
All	All	2664/2704 (98%)	2576 (97%)	81 (3%)	7 (0%)	46	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	384	ALA
2	E	384	ALA
2	G	384	ALA
2	I	384	ALA
1	A	285	THR
1	D	285	THR
1	H	285	THR

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	215/217 (99%)	210 (98%)	5 (2%)	58	87
1	D	215/217 (99%)	210 (98%)	5 (2%)	58	87
1	F	215/217 (99%)	210 (98%)	5 (2%)	58	87
1	H	215/217 (99%)	210 (98%)	5 (2%)	58	87
2	B	296/298 (99%)	289 (98%)	7 (2%)	57	86
2	E	296/298 (99%)	289 (98%)	7 (2%)	57	86
2	G	296/298 (99%)	287 (97%)	9 (3%)	48	83
2	I	296/298 (99%)	288 (97%)	8 (3%)	52	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2044/2060 (99%)	1993 (98%)	51 (2%)	55 85

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LYS
1	A	117	ARG
1	A	156	LEU
1	A	255	LYS
1	A	274	ARG
2	B	95	GLN
2	B	175	GLN
2	B	258	ASN
2	B	287	LEU
2	B	319	PHE
2	B	322	ILE
2	B	348	ARG
1	D	90	LYS
1	D	117	ARG
1	D	156	LEU
1	D	255	LYS
1	D	274	ARG
2	E	95	GLN
2	E	175	GLN
2	E	258	ASN
2	E	287	LEU
2	E	319	PHE
2	E	322	ILE
2	E	348	ARG
1	F	90	LYS
1	F	117	ARG
1	F	156	LEU
1	F	255	LYS
1	F	274	ARG
2	G	95	GLN
2	G	158	TYR
2	G	175	GLN
2	G	200	PRO
2	G	258	ASN
2	G	287	LEU
2	G	319	PHE
2	G	322	ILE

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Mol	Chain	Res	Type
2	G	348	ARG
1	H	90	LYS
1	H	117	ARG
1	H	156	LEU
1	H	255	LYS
1	H	274	ARG
2	I	95	GLN
2	I	175	GLN
2	I	200	PRO
2	I	258	ASN
2	I	287	LEU
2	I	319	PHE
2	I	322	ILE
2	I	348	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	HIS
2	B	94	ASN
2	B	95	GLN
2	B	342	ASN
2	B	352	ASN
2	E	94	ASN
2	E	95	GLN
2	E	342	ASN
2	E	352	ASN
2	G	50	HIS
2	G	94	ASN
2	G	95	GLN
2	G	342	ASN
2	G	352	ASN
2	I	94	ASN
2	I	95	GLN
2	I	342	ASN
2	I	352	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	NEP	A	246	1	10,14,15	1.54	2 (20%)	4,20,22	1.17	0
1	NEP	D	246	1	10,14,15	1.49	3 (30%)	4,20,22	1.19	0
1	NEP	F	246	1	10,14,15	1.43	2 (20%)	4,20,22	1.20	0
1	NEP	H	246	1	10,14,15	1.59	2 (20%)	4,20,22	1.24	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	NEP	A	246	1	-	0/4/12/14	0/1/1/1
1	NEP	D	246	1	-	0/4/12/14	0/1/1/1
1	NEP	F	246	1	-	0/4/12/14	0/1/1/1
1	NEP	H	246	1	-	0/4/12/14	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	246	NEP	P-O1P	-3.36	1.47	1.54
1	H	246	NEP	P-O2P	-3.30	1.47	1.54
1	A	246	NEP	P-O1P	-3.15	1.47	1.54
1	H	246	NEP	P-O1P	-3.07	1.48	1.54
1	A	246	NEP	P-O2P	-2.80	1.48	1.54
1	D	246	NEP	P-O1P	-2.77	1.48	1.54
1	D	246	NEP	P-O2P	-2.35	1.49	1.54
1	F	246	NEP	P-O2P	-2.06	1.50	1.54
1	D	246	NEP	P-O3P	2.30	1.49	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	246	NEP	1	0
1	D	246	NEP	1	0
1	F	246	NEP	1	0
1	H	246	NEP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
4	COA	A	300	-	40,50,50	0.78	1 (2%)	50,75,75	1.46	8 (16%)
3	SO4	B	389	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	B	390	-	4,4,4	0.31	0	6,6,6	0.16	0
4	COA	D	301	-	40,50,50	0.69	0	50,75,75	1.61	9 (18%)
3	SO4	E	389	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	E	390	-	4,4,4	0.09	0	6,6,6	0.08	0
4	COA	F	400	-	40,50,50	0.73	0	50,75,75	1.99	10 (20%)
3	SO4	G	389	-	4,4,4	0.32	0	6,6,6	0.21	0
3	SO4	G	390	-	4,4,4	0.42	0	6,6,6	0.25	0
4	COA	H	401	-	40,50,50	0.70	1 (2%)	50,75,75	2.06	11 (22%)
3	SO4	I	389	-	4,4,4	0.60	0	6,6,6	0.12	0
3	SO4	I	390	-	4,4,4	0.14	0	6,6,6	0.15	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
4	COA	A	300	-	-	0/44/64/64	0/3/3/3
3	SO4	B	389	-	-	0/0/0/0	0/0/0/0
3	SO4	B	390	-	-	0/0/0/0	0/0/0/0
4	COA	D	301	-	-	0/44/64/64	0/3/3/3
3	SO4	E	389	-	-	0/0/0/0	0/0/0/0
3	SO4	E	390	-	-	0/0/0/0	0/0/0/0
4	COA	F	400	-	-	0/44/64/64	0/3/3/3
3	SO4	G	389	-	-	0/0/0/0	0/0/0/0
3	SO4	G	390	-	-	0/0/0/0	0/0/0/0
4	COA	H	401	-	-	0/44/64/64	0/3/3/3
3	SO4	I	389	-	-	0/0/0/0	0/0/0/0
3	SO4	I	390	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	401	COA	C6P-C5P	2.18	1.55	1.51
4	A	300	COA	OAP-CAP	2.90	1.48	1.42

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	400	COA	OAP-CAP-C9P	-4.58	99.88	110.38
4	F	400	COA	C2P-C3P-N4P	-4.38	103.73	112.37
4	H	401	COA	O5P-C5P-N4P	-4.31	114.38	122.94
4	H	401	COA	C3P-N4P-C5P	-4.21	114.51	122.79
4	H	401	COA	P2A-O3A-P1A	-3.82	122.01	132.73
4	H	401	COA	C2P-C3P-N4P	-3.80	104.87	112.37
4	A	300	COA	P2A-O3A-P1A	-3.79	122.08	132.73
4	F	400	COA	P2A-O3A-P1A	-3.60	122.63	132.73
4	D	301	COA	P2A-O3A-P1A	-3.59	122.64	132.73
4	H	401	COA	OAP-CAP-C9P	-3.49	102.37	110.38
4	F	400	COA	O5P-C5P-C6P	-3.45	116.04	121.98
4	D	301	COA	OAP-CAP-C9P	-3.28	102.85	110.38
4	F	400	COA	C1B-N9A-C4A	-3.24	122.06	126.94
4	H	401	COA	C1B-N9A-C4A	-3.08	122.30	126.94
4	A	300	COA	CEP-CBP-CCP	-2.88	104.77	108.50
4	D	301	COA	C2P-C3P-N4P	-2.87	106.71	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	301	COA	CAP-C9P-N8P	-2.74	110.39	116.47
4	F	400	COA	CEP-CBP-CCP	-2.72	104.98	108.50
4	A	300	COA	C7P-C6P-C5P	-2.60	108.03	112.31
4	H	401	COA	O5P-C5P-C6P	-2.51	117.65	121.98
4	D	301	COA	O5P-C5P-C6P	-2.36	117.92	121.98
4	A	300	COA	C1B-N9A-C4A	-2.32	123.45	126.94
4	D	301	COA	C1B-N9A-C4A	-2.14	123.72	126.94
4	A	300	COA	O5P-C5P-C6P	-2.09	118.38	121.98
4	A	300	COA	OAP-CAP-C9P	-2.00	105.78	110.38
4	H	401	COA	O9A-P3B-O8A	2.05	115.17	107.38
4	D	301	COA	CEP-CBP-CAP	2.14	113.25	109.34
4	F	400	COA	O6A-CCP-CBP	2.15	114.01	110.55
4	H	401	COA	CEP-CBP-CAP	2.55	114.00	109.34
4	D	301	COA	C6P-C5P-N4P	2.65	121.07	116.46
4	A	300	COA	CEP-CBP-CAP	2.91	114.66	109.34
4	F	400	COA	C6P-C5P-N4P	3.43	122.43	116.46
4	A	300	COA	C2B-C1B-N9A	4.44	121.08	114.29
4	F	400	COA	C2B-C1B-N9A	5.22	122.26	114.29
4	F	400	COA	CDP-CBP-CCP	5.45	115.57	108.50
4	D	301	COA	C2B-C1B-N9A	5.50	122.70	114.29
4	H	401	COA	C2B-C1B-N9A	6.03	123.50	114.29
4	H	401	COA	C6P-C5P-N4P	6.62	127.97	116.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	300	COA	1	0
3	B	389	SO4	1	0
4	D	301	COA	5	0
4	H	401	COA	3	0

5.7 Other polymers (i)

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	285/288 (98%)	-0.31	1 (0%) 93 92	18, 35, 51, 59	0
1	D	285/288 (98%)	-0.28	1 (0%) 93 92	19, 37, 51, 60	0
1	F	285/288 (98%)	-0.33	1 (0%) 93 92	18, 34, 50, 59	0
1	H	285/288 (98%)	-0.32	0 100 100	19, 36, 51, 60	0
2	B	385/388 (99%)	-0.12	12 (3%) 52 45	18, 36, 64, 79	0
2	E	385/388 (99%)	-0.10	7 (1%) 71 68	19, 37, 64, 78	0
2	G	385/388 (99%)	-0.15	11 (2%) 55 49	19, 37, 64, 78	0
2	I	385/388 (99%)	-0.08	14 (3%) 46 38	19, 37, 65, 79	0
All	All	2680/2704 (99%)	-0.19	47 (1%) 71 68	18, 36, 60, 79	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	322	ILE	6.2
2	I	322	ILE	5.3
2	I	324	ARG	4.0
2	E	132	GLU	3.7
2	I	132	GLU	3.5
2	G	322	ILE	3.4
2	G	363	ASP	3.3
2	I	323	VAL	3.3
2	B	321	GLY	3.1
2	E	342	ASN	3.1
2	I	309	ASP	3.0
2	I	138	GLU	3.0
2	G	362	ALA	2.9
2	B	138	GLU	2.7
2	I	325	CYS	2.7
2	I	321	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	223	GLU	2.7
2	I	139	GLU	2.6
2	B	309	ASP	2.6
2	E	372	LYS	2.6
2	B	310	LYS	2.6
2	G	321	GLY	2.5
2	E	364	SER	2.5
2	I	352	ASN	2.5
2	B	84	TYR	2.4
2	G	88	ALA	2.3
2	B	139	GLU	2.3
2	B	89	ASN	2.3
2	B	140	THR	2.2
2	G	256	ASP	2.2
1	F	223	GLU	2.2
2	I	365	GLY	2.2
2	B	175	GLN	2.2
2	I	355	GLU	2.2
2	G	84	TYR	2.2
1	A	6	LYS	2.1
2	G	372	LYS	2.1
2	E	355	GLU	2.1
2	B	312	LYS	2.1
2	G	260	GLY	2.1
2	E	84	TYR	2.1
2	I	353	ASN	2.1
2	G	320	GLY	2.0
2	B	56	LYS	2.0
2	G	64	ASN	2.0
2	E	256	ASP	2.0
2	I	364	SER	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	NEP	H	246	14/15	0.98	0.11	-	29,32,36,36	0
1	NEP	F	246	14/15	0.96	0.12	-	27,33,34,34	0
1	NEP	A	246	14/15	0.97	0.10	-	29,32,35,36	0
1	NEP	D	246	14/15	0.96	0.13	-	30,33,38,38	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	SO4	I	389	5/5	0.73	0.41	5.08	68,68,68,69	5
3	SO4	B	390	5/5	0.95	0.16	0.42	53,53,54,55	0
3	SO4	B	389	5/5	0.87	0.23	0.42	28,29,30,30	5
4	COA	D	301	48/48	0.95	0.17	0.22	43,46,53,54	0
3	SO4	G	389	5/5	0.93	0.20	0.19	22,23,24,25	5
4	COA	F	400	48/48	0.95	0.16	0.07	39,45,47,50	0
4	COA	A	300	48/48	0.94	0.16	-0.03	43,48,52,53	0
3	SO4	G	390	5/5	0.95	0.17	-0.07	68,68,69,69	0
4	COA	H	401	48/48	0.96	0.15	-0.14	33,44,58,59	0
3	SO4	I	390	5/5	0.96	0.17	-0.31	55,56,56,57	0
3	SO4	E	389	5/5	0.95	0.15	-0.69	28,29,30,31	5
3	SO4	E	390	5/5	0.98	0.20	-	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.