Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:18 AM GMT

PDB ID	:	3A77
Title	:	The crystal structure of phosphorylated IRF-3
Authors	:	Takahasi, K.; Horiuchi, M.; Noda, N.N.; Inagaki, F.
Deposited on	:	2009-09-17
Resolution	:	1.80 Å(reported)

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

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

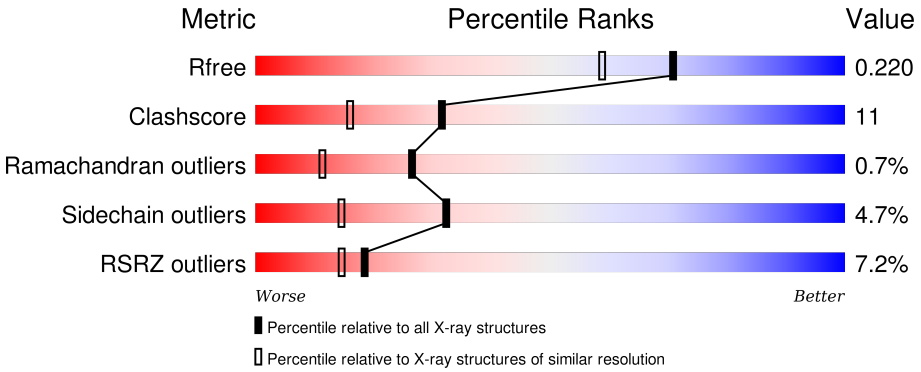
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	242	4% 83% 11%
1	B	242	7% 76% 19%
1	C	242	7% 74% 21%
1	D	242	10% 69% 21% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	A	2001	-	-	-	X
2	ACY	C	2003	-	-	-	X
3	MPD	A	3002	-	-	-	X
3	MPD	B	3001	-	-	-	X
3	MPD	C	3003	-	-	-	X
3	MPD	D	3004	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8328 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.

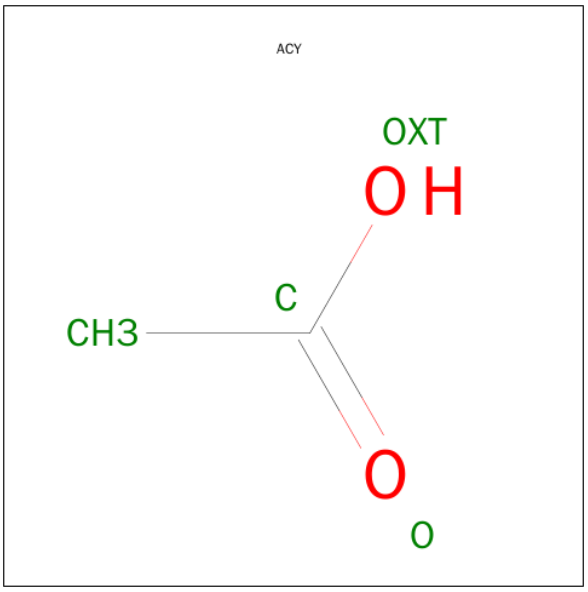
- Molecule 1 is a protein called Interferon regulatory factor 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	P	S	0	0	0
			1824	1161	312	339	2	10			
1	B	234	Total	C	N	O	P	S	0	0	0
			1836	1168	314	342	2	10			
1	C	233	Total	C	N	O	P	S	0	0	0
			1816	1157	308	339	2	10			
1	D	230	Total	C	N	O	P	S	0	0	0
			1805	1151	309	333	2	10			

There are 12 discrepancies between the modelled and reference sequences:

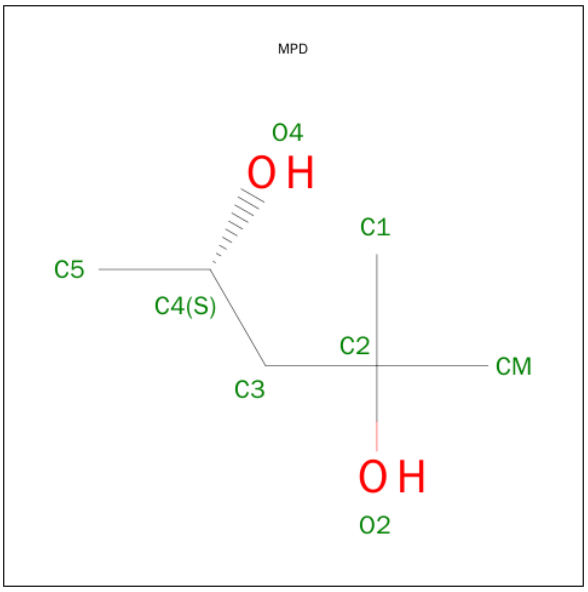
Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLY	-	EXPRESSION TAG	UNP Q14653
A	187	ALA	-	EXPRESSION TAG	UNP Q14653
A	188	MET	-	EXPRESSION TAG	UNP Q14653
B	186	GLY	-	EXPRESSION TAG	UNP Q14653
B	187	ALA	-	EXPRESSION TAG	UNP Q14653
B	188	MET	-	EXPRESSION TAG	UNP Q14653
C	186	GLY	-	EXPRESSION TAG	UNP Q14653
C	187	ALA	-	EXPRESSION TAG	UNP Q14653
C	188	MET	-	EXPRESSION TAG	UNP Q14653
D	186	GLY	-	EXPRESSION TAG	UNP Q14653
D	187	ALA	-	EXPRESSION TAG	UNP Q14653
D	188	MET	-	EXPRESSION TAG	UNP Q14653

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

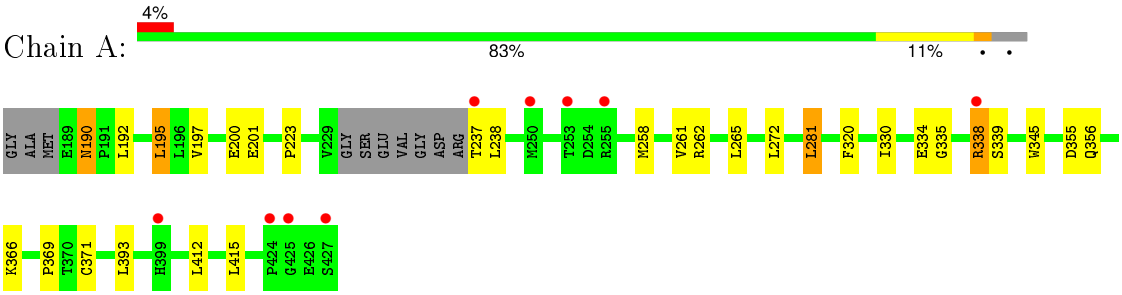
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	266	Total O 266 266	0	0
4	B	275	Total O 275 275	0	0
4	C	254	Total O 254 254	0	0
4	D	212	Total O 212 212	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

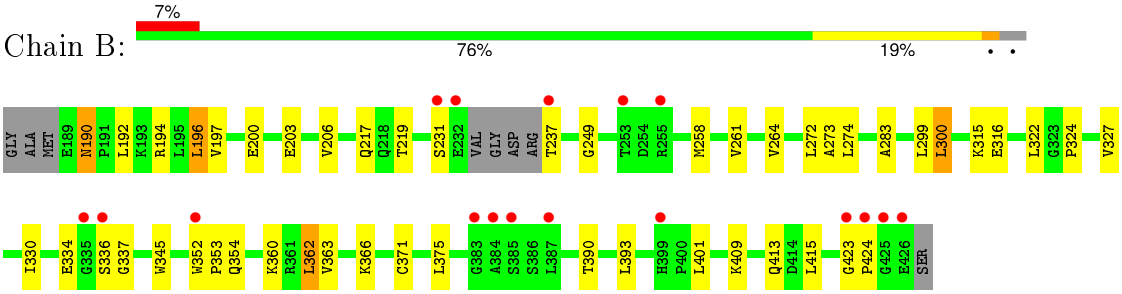
- Molecule 1: Interferon regulatory factor 3

Chain A:



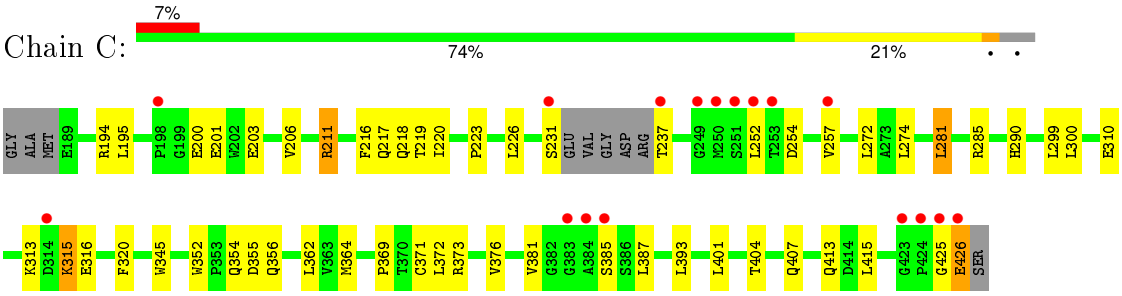
- Molecule 1: Interferon regulatory factor 3

Chain B:



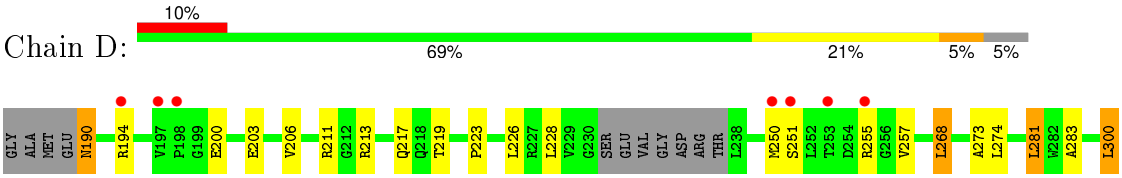
- Molecule 1: Interferon regulatory factor 3

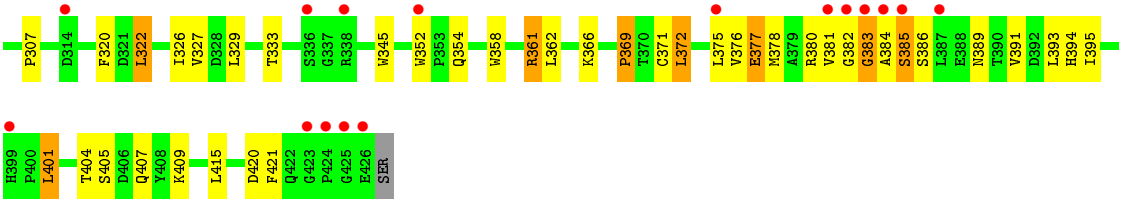
Chain C:



- Molecule 1: Interferon regulatory factor 3

Chain D:




P307
D314
F320
D321
L322
I326
V327
D328
L329
T333
S336
G337
R338
W345
W352
P353
Q354
W358
R361
L362
K366
P369
T370
C371
L372
L375
V376
E377
M378
A379
R380
V381
G382
G383
A384
S385
S386
L387
E388
N389
T390
V391
D392
L393
H394
I395
H399
P400
L401
T404
S405
D406
Q407
Y408
K409
L415
D420
F421
Q422
G423
P424
G425
E426
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.47Å 102.46Å 68.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.7 (20.00-1.80) 97.5 (19.94-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.221 0.194 , 0.220	Depositor DCC
R_{free} test set	10499 reflections (10.00%)	DCC
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.8	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 107221 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8328	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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: ACY, MPD, SEP

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	0.30	0/1855	0.59	1/2524 (0.0%)
1	B	0.31	0/1867	0.60	1/2541 (0.0%)
1	C	0.30	0/1846	0.58	0/2514
1	D	0.30	0/1836	0.60	1/2499 (0.0%)
All	All	0.30	0/7404	0.59	3/10078 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	PRO	N-CA-C	-5.20	98.57	112.10
1	D	369	PRO	N-CA-C	-5.18	98.62	112.10
1	B	300	LEU	CA-CB-CG	5.09	127.01	115.30

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	1824	0	1756	20	0
1	B	1836	0	1765	37	0
1	C	1816	0	1743	48	0
1	D	1805	0	1739	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	3	0	0
2	C	4	0	3	0	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
3	C	8	0	14	1	0
3	D	8	0	14	0	0
4	A	266	0	0	2	0
4	B	275	0	0	5	0
4	C	254	0	0	5	0
4	D	212	0	0	1	0
All	All	8328	0	7065	154	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 11.

All (154) 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:B:264:VAL:HG21	1:B:363:VAL:HG21	1.52	0.91
1:D:405:SER:O	1:D:409:LYS:HD3	1.72	0.90
3:B:3001:MPD:H13	3:B:3001:MPD:O4	1.84	0.77
1:B:352:TRP:HE1	1:B:354:GLN:HE21	1.33	0.76
3:C:3003:MPD:H13	3:C:3003:MPD:O4	1.84	0.74
1:A:261:VAL:O	1:A:265:LEU:HD13	1.90	0.72
1:B:261:VAL:O	1:B:264:VAL:HG22	1.90	0.72
1:B:409:LYS:O	1:B:413:GLN:HG3	1.91	0.71
1:A:237:THR:HG21	1:C:237:THR:HG23	1.73	0.70
1:C:352:TRP:NE1	1:C:354:GLN:HG3	2.08	0.69
1:A:223:PRO:HG2	1:D:223:PRO:HG2	1.75	0.69
1:B:352:TRP:CE3	1:B:353:PRO:HD2	2.29	0.68
1:A:330:ILE:O	1:A:334:GLU:HG2	1.95	0.67
1:C:216:PHE:HZ	1:C:218:GLN:HE21	1.44	0.65
1:C:300:LEU:HD21	1:C:364:MET:HG3	1.78	0.65
1:B:324:PRO:HA	1:B:327:VAL:HG22	1.79	0.64
1:D:404:THR:HG23	1:D:407:GLN:HE21	1.61	0.64
1:C:252:LEU:HD23	1:C:257:VAL:HG13	1.79	0.63
1:D:213:ARG:HB2	1:D:213:ARG:NH2	2.12	0.63
1:C:254:ASP:HB3	1:C:257:VAL:HG12	1.80	0.63
1:C:425:GLY:O	1:C:426:GLU:HB3	1.99	0.63
1:A:237:THR:CG2	1:C:237:THR:HG23	2.28	0.63
1:D:404:THR:OG1	1:D:407:GLN:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LYS:HE2	1:D:420:ASP:OD1	2.00	0.62
1:B:237:THR:HG21	4:B:1581:HOH:O	1.99	0.61
1:D:203:GLU:HG3	1:D:219:THR:CG2	2.31	0.60
1:D:333:THR:HB	1:D:409:LYS:HE3	1.83	0.60
1:D:281:LEU:HB2	1:D:320:PHE:HB3	1.83	0.59
1:C:385:SER:HB3	1:C:387:LEU:HD23	1.87	0.57
1:A:237:THR:OG1	1:A:238:LEU:HD22	2.05	0.56
1:D:300:LEU:HD22	1:D:345:TRP:CZ3	2.41	0.56
1:C:203:GLU:HG3	1:C:219:THR:CG2	2.37	0.55
1:D:194:ARG:O	1:D:200:GLU:HG3	2.06	0.55
1:D:381:VAL:HG12	1:D:381:VAL:O	2.07	0.55
1:A:201:GLU:OE1	1:A:223:PRO:HG3	2.06	0.55
1:D:371:CYS:SG	1:D:372:LEU:HD13	2.47	0.54
1:C:231:SER:HB3	4:C:2016:HOH:O	2.08	0.54
1:B:190:ASN:C	1:B:190:ASN:HD22	2.10	0.53
1:A:281:LEU:HB2	1:A:320:PHE:HB3	1.90	0.52
1:B:194:ARG:HD2	4:B:1398:HOH:O	2.10	0.52
1:B:371:CYS:HB3	1:B:393:LEU:O	2.09	0.52
1:B:324:PRO:HA	1:B:327:VAL:CG2	2.39	0.52
1:A:335:GLY:HA2	4:A:2051:HOH:O	2.10	0.52
1:B:197:VAL:CG2	1:B:200:GLU:HG2	2.39	0.52
1:C:371:CYS:HB3	1:C:393:LEU:O	2.09	0.52
1:C:203:GLU:HG3	1:C:219:THR:HG23	1.92	0.51
1:B:194:ARG:HH11	1:B:194:ARG:HG2	1.76	0.51
1:B:352:TRP:CD2	1:B:353:PRO:HD2	2.45	0.51
1:D:211:ARG:HD2	1:D:257:VAL:HG21	1.91	0.51
1:D:255:ARG:HH21	1:D:255:ARG:HG3	1.76	0.51
1:C:371:CYS:SG	1:C:372:LEU:HD13	2.51	0.50
1:B:390:THR:HA	1:B:401:LEU:O	2.10	0.50
1:C:216:PHE:HZ	1:C:218:GLN:NE2	2.10	0.50
1:C:376:VAL:CG2	4:C:1470:HOH:O	2.59	0.50
1:C:404:THR:OG1	1:C:407:GLN:HG3	2.11	0.50
1:C:194:ARG:O	1:C:200:GLU:HG3	2.12	0.49
1:C:413:GLN:HG2	4:C:1961:HOH:O	2.13	0.49
1:D:382:GLY:O	1:D:383:GLY:C	2.51	0.49
1:D:352:TRP:HB3	1:D:354:GLN:OE1	2.12	0.49
1:D:371:CYS:HB3	1:D:393:LEU:O	2.13	0.48
1:A:190:ASN:C	1:A:190:ASN:HD22	2.15	0.48
1:C:290:HIS:HD2	1:C:310:GLU:OE1	1.97	0.48
1:D:190:ASN:C	1:D:190:ASN:HD22	2.17	0.48
1:C:315:LYS:HD3	1:C:316:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ARG:O	1:C:313:LYS:HG3	2.12	0.48
1:A:338:ARG:HD2	1:A:339:SER:O	2.14	0.48
1:C:401:LEU:N	1:C:401:LEU:HD22	2.29	0.48
1:B:345:TRP:CZ2	1:B:366:LYS:HD3	2.49	0.47
1:C:369:PRO:CG	1:C:372:LEU:HD22	2.44	0.47
1:C:281:LEU:HB2	1:C:320:PHE:HB3	1.94	0.47
1:D:404:THR:H	1:D:407:GLN:HE21	1.61	0.47
1:D:391:VAL:O	1:D:401:LEU:HD23	2.13	0.47
1:D:377:GLU:O	1:D:381:VAL:HG23	2.15	0.47
1:D:307:PRO:HB3	1:D:358:TRP:CE3	2.49	0.47
1:A:371:CYS:HB3	1:A:393:LEU:O	2.15	0.47
1:C:387:LEU:HD22	1:C:387:LEU:N	2.30	0.47
1:D:401:LEU:HD23	1:D:401:LEU:N	2.29	0.47
1:C:299:LEU:HG	4:C:1982:HOH:O	2.12	0.47
1:B:249:GLY:HA2	1:B:258:MET:CE	2.44	0.47
1:D:385:SER:HB2	1:D:405:SER:HB2	1.96	0.47
1:B:316:GLU:HG2	4:B:1590:HOH:O	2.14	0.47
1:D:401:LEU:H	1:D:401:LEU:HD23	1.79	0.47
1:C:274:LEU:HD13	1:C:274:LEU:C	2.35	0.46
1:D:376:VAL:O	1:D:380:ARG:HG3	2.16	0.46
1:D:394:HIS:HE1	4:D:1269:HOH:O	1.97	0.45
1:B:274:LEU:C	1:B:274:LEU:HD13	2.37	0.45
1:C:352:TRP:HE1	1:C:354:GLN:HG3	1.82	0.45
1:C:218:GLN:CD	1:C:220:ILE:HD11	2.36	0.45
1:B:324:PRO:O	1:B:327:VAL:HG22	2.16	0.45
1:D:345:TRP:CZ2	1:D:366:LYS:HD3	2.52	0.45
1:B:352:TRP:CD1	1:B:354:GLN:HB2	2.52	0.45
1:D:393:LEU:O	1:D:395:ILE:HG23	2.17	0.45
1:C:254:ASP:HB3	1:C:257:VAL:CG1	2.46	0.45
1:D:369:PRO:HB2	1:D:372:LEU:HD22	1.99	0.45
1:A:345:TRP:CZ2	1:A:366:LYS:HD3	2.52	0.45
1:A:195:LEU:HD13	1:A:393:LEU:HD13	1.98	0.44
1:D:380:ARG:HG2	1:D:380:ARG:HH21	1.82	0.44
1:D:329:LEU:O	1:D:333:THR:HG23	2.18	0.44
1:D:404:THR:H	1:D:407:GLN:NE2	2.14	0.44
1:D:274:LEU:HD13	1:D:274:LEU:C	2.38	0.44
1:D:213:ARG:CB	1:D:213:ARG:NH2	2.79	0.44
1:C:194:ARG:HD2	4:C:1731:HOH:O	2.17	0.44
1:C:425:GLY:O	1:C:426:GLU:CB	2.65	0.44
1:D:226:LEU:HD12	1:D:226:LEU:C	2.38	0.44
1:C:387:LEU:HD22	1:C:387:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASN:ND2	1:B:192:LEU:H	2.15	0.44
1:D:206:VAL:O	1:D:217:GLN:HA	2.18	0.44
1:B:360:LYS:HB3	1:B:362:LEU:HD13	1.99	0.44
1:C:315:LYS:HD2	1:C:315:LYS:C	2.38	0.44
1:C:206:VAL:O	1:C:217:GLN:HA	2.17	0.44
1:B:197:VAL:CG2	1:B:200:GLU:CG	2.97	0.43
1:B:330:ILE:O	1:B:334:GLU:HG3	2.18	0.43
1:B:203:GLU:HG3	1:B:219:THR:CG2	2.47	0.43
1:C:272:LEU:HD13	1:C:272:LEU:C	2.39	0.43
1:D:213:ARG:CB	1:D:213:ARG:HH21	2.31	0.43
1:D:203:GLU:CG	1:D:219:THR:CG2	2.96	0.43
1:D:380:ARG:C	1:D:382:GLY:H	2.21	0.43
1:D:213:ARG:HB2	1:D:213:ARG:CZ	2.48	0.43
1:D:378:MET:CE	1:D:391:VAL:HB	2.49	0.43
1:D:322:LEU:HD22	1:D:326:ILE:HG12	2.00	0.43
1:C:226:LEU:C	1:C:226:LEU:HD12	2.39	0.42
1:D:358:TRP:O	1:D:361:ARG:HD2	2.19	0.42
1:C:369:PRO:HG3	1:C:372:LEU:HD22	2.01	0.42
1:B:206:VAL:O	1:B:217:GLN:HA	2.19	0.42
1:C:211:ARG:HG2	1:C:362:LEU:HD22	2.02	0.42
1:C:373:ARG:O	1:C:376:VAL:HG22	2.20	0.42
1:B:336:SER:HB2	4:B:1761:HOH:O	2.18	0.42
1:C:355:ASP:O	1:C:356:GLN:C	2.58	0.42
1:B:231:SER:HA	4:B:2011:HOH:O	2.20	0.42
1:C:218:GLN:OE1	1:C:220:ILE:HD11	2.20	0.42
1:D:273:ALA:O	1:D:283:ALA:HA	2.20	0.42
1:D:385:SER:O	1:D:386:SEP:HB3	2.20	0.41
1:D:381:VAL:HG12	1:D:389:ASN:ND2	2.34	0.41
1:D:404:THR:HG23	1:D:407:GLN:NE2	2.30	0.41
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.90	0.41
1:C:385:SER:HB3	1:C:387:LEU:CD2	2.50	0.41
4:A:1866:HOH:O	1:B:423:GLY:HA3	2.21	0.41
1:B:196:LEU:HD11	1:B:322:LEU:HD23	2.01	0.41
1:B:272:LEU:C	1:B:272:LEU:HD13	2.41	0.41
1:C:300:LEU:HD23	1:C:345:TRP:CZ3	2.55	0.41
1:A:190:ASN:ND2	1:A:192:LEU:H	2.19	0.41
1:A:258:MET:O	1:A:262:ARG:HG3	2.20	0.41
1:B:194:ARG:NH1	1:B:194:ARG:HG2	2.33	0.41
1:A:355:ASP:O	1:A:356:GLN:C	2.59	0.41
1:C:201:GLU:OE2	1:C:223:PRO:HG3	2.21	0.41
1:A:281:LEU:HA	1:A:281:LEU:HD12	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:C	1:A:272:LEU:HD13	2.42	0.40
1:B:261:VAL:O	1:B:264:VAL:CG2	2.65	0.40
1:C:290:HIS:CE1	1:D:421:PHE:O	2.74	0.40
1:A:197:VAL:CG2	1:A:200:GLU:HG2	2.51	0.40
1:B:261:VAL:HA	1:B:264:VAL:HG22	2.03	0.40
1:B:194:ARG:O	1:B:200:GLU:HG3	2.21	0.40
1:D:307:PRO:HB3	1:D:358:TRP:CZ3	2.56	0.40
1:B:273:ALA:O	1:B:283:ALA:HA	2.22	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	226/242 (93%)	222 (98%)	4 (2%)	0	100 100
1	B	228/242 (94%)	222 (97%)	4 (2%)	2 (1%)	21 7
1	C	227/242 (94%)	222 (98%)	5 (2%)	0	100 100
1	D	224/242 (93%)	214 (96%)	6 (3%)	4 (2%)	11 2
All	All	905/968 (94%)	880 (97%)	19 (2%)	6 (1%)	26 11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	384	ALA
1	B	337	GLY
1	D	383	GLY
1	D	385	SER
1	D	251	SER
1	B	424	PRO

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	194/201 (96%)	188 (97%)	6 (3%)	47 30
1	B	195/201 (97%)	187 (96%)	8 (4%)	37 19
1	C	192/201 (96%)	185 (96%)	7 (4%)	42 24
1	D	191/201 (95%)	176 (92%)	15 (8%)	15 4
All	All	772/804 (96%)	736 (95%)	36 (5%)	32 14

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	195	LEU
1	A	281	LEU
1	A	338	ARG
1	A	412	LEU
1	A	415	LEU
1	B	190	ASN
1	B	196	LEU
1	B	299	LEU
1	B	300	LEU
1	B	315	LYS
1	B	362	LEU
1	B	375	LEU
1	B	415	LEU
1	C	195	LEU
1	C	211	ARG
1	C	281	LEU
1	C	315	LYS
1	C	381	VAL
1	C	415	LEU
1	C	426	GLU
1	D	190	ASN
1	D	228	LEU
1	D	250	MET

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Mol	Chain	Res	Type
1	D	268	LEU
1	D	281	LEU
1	D	300	LEU
1	D	322	LEU
1	D	327	VAL
1	D	361	ARG
1	D	362	LEU
1	D	372	LEU
1	D	375	LEU
1	D	377	GLU
1	D	401	LEU
1	D	415	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	214	GLN
1	A	217	GLN
1	A	302	ASN
1	A	413	GLN
1	A	422	GLN
1	B	190	ASN
1	B	214	GLN
1	B	354	GLN
1	B	413	GLN
1	B	422	GLN
1	C	214	GLN
1	C	218	GLN
1	C	290	HIS
1	C	422	GLN
1	D	190	ASN
1	D	214	GLN
1	D	284	GLN
1	D	288	HIS
1	D	389	ASN
1	D	394	HIS
1	D	407	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 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	SEP	A	386	1	8,9,10	0.97	0	8,12,14	0.90	0
1	SEP	A	402	1	8,9,10	1.07	0	8,12,14	1.01	0
1	SEP	B	386	1	8,9,10	1.08	0	8,12,14	1.41	1 (12%)
1	SEP	B	402	1	8,9,10	1.14	1 (12%)	8,12,14	1.24	1 (12%)
1	SEP	C	386	1	8,9,10	1.11	0	8,12,14	1.44	1 (12%)
1	SEP	C	402	1	8,9,10	1.12	0	8,12,14	1.46	1 (12%)
1	SEP	D	386	1	8,9,10	1.28	2 (25%)	8,12,14	1.89	1 (12%)
1	SEP	D	402	1	8,9,10	1.14	1 (12%)	8,12,14	1.33	1 (12%)

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	SEP	A	386	1	-	0/6/8/10	0/0/0/0
1	SEP	A	402	1	-	0/6/8/10	0/0/0/0
1	SEP	B	386	1	-	0/6/8/10	0/0/0/0
1	SEP	B	402	1	-	0/6/8/10	0/0/0/0
1	SEP	C	386	1	-	0/6/8/10	0/0/0/0
1	SEP	C	402	1	-	0/6/8/10	0/0/0/0
1	SEP	D	386	1	-	0/6/8/10	0/0/0/0
1	SEP	D	402	1	-	0/6/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	SEP	P-O2P	2.02	1.62	1.54
1	D	386	SEP	P-O2P	2.08	1.62	1.54
1	D	402	SEP	P-O2P	2.08	1.62	1.54
1	D	386	SEP	P-O3P	2.15	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	402	SEP	OG-CB-CA	2.21	110.16	108.27
1	D	402	SEP	OG-CB-CA	2.56	110.46	108.27
1	B	386	SEP	OG-CB-CA	2.98	110.81	108.27
1	C	386	SEP	OG-CB-CA	3.13	110.94	108.27
1	C	402	SEP	OG-CB-CA	3.15	110.96	108.27
1	D	386	SEP	OG-CB-CA	4.53	112.14	108.27

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
1	D	386	SEP	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	$\#\|Z\| > 2$
2	ACY	A	2001	-	1,3,3	1.59	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MPD	A	3002	-	6,7,7	0.39	0	7,10,10	0.44	0
3	MPD	B	3001	-	6,7,7	0.63	0	7,10,10	3.13	4 (57%)
2	ACY	C	2003	-	1,3,3	1.71	0	0,3,3	0.00	-
3	MPD	C	3003	-	6,7,7	0.64	0	7,10,10	3.12	4 (57%)
3	MPD	D	3004	-	6,7,7	0.40	0	7,10,10	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACY	A	2001	-	-	0/0/0/0	0/0/0/0
3	MPD	A	3002	-	-	0/5/5/5	0/0/0/0
3	MPD	B	3001	-	-	0/5/5/5	0/0/0/0
2	ACY	C	2003	-	-	0/0/0/0	0/0/0/0
3	MPD	C	3003	-	-	0/5/5/5	0/0/0/0
3	MPD	D	3004	-	-	0/5/5/5	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})
3	B	3001	MPD	CM-C2-C3	-4.69	82.75	109.90
3	C	3003	MPD	CM-C2-C3	-4.65	82.98	109.90
3	C	3003	MPD	C1-C2-C3	-3.60	89.03	109.90
3	B	3001	MPD	C1-C2-C3	-3.60	89.06	109.90
3	C	3003	MPD	O2-C2-CM	2.93	118.82	108.09
3	B	3001	MPD	O2-C2-CM	2.94	118.89	108.09
3	B	3001	MPD	O2-C2-C1	4.75	125.52	108.09
3	C	3003	MPD	O2-C2-C1	4.80	125.68	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3001	MPD	1	0
3	C	3003	MPD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	230/242 (95%)	0.10	9 (3%) 43 37	10, 16, 36, 47	0
1	B	232/242 (95%)	0.20	17 (7%) 18 14	9, 16, 42, 63	0
1	C	231/242 (95%)	0.27	17 (7%) 17 14	11, 20, 43, 57	0
1	D	228/242 (94%)	0.49	23 (10%) 9 7	11, 20, 46, 64	0
All	All	921/968 (95%)	0.26	66 (7%) 18 14	9, 18, 43, 64	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	ALA	9.6
1	D	425	GLY	8.2
1	D	423	GLY	7.0
1	C	231	SER	6.1
1	B	424	PRO	6.1
1	D	385	SER	5.6
1	D	424	PRO	5.2
1	C	237	THR	5.1
1	D	381	VAL	4.6
1	B	425	GLY	4.6
1	A	427	SER	4.4
1	B	237	THR	4.3
1	C	249	GLY	4.3
1	C	250	MET	4.1
1	B	423	GLY	4.1
1	B	231	SER	4.0
1	D	253	THR	4.0
1	A	425	GLY	3.9
1	B	426	GLU	3.8
1	B	336	SER	3.7
1	C	253	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	382	GLY	3.6
1	B	335	GLY	3.5
1	C	423	GLY	3.5
1	A	255	ARG	3.5
1	C	384	ALA	3.5
1	B	383	GLY	3.3
1	C	252	LEU	3.3
1	D	336	SER	3.3
1	D	198	PRO	3.2
1	D	426	GLU	3.2
1	C	426	GLU	3.1
1	C	425	GLY	3.1
1	A	237	THR	3.1
1	D	255	ARG	3.1
1	D	338	ARG	2.9
1	D	352	TRP	2.9
1	C	385	SER	2.9
1	D	250	MET	2.9
1	D	197	VAL	2.9
1	C	424	PRO	2.8
1	B	253	THR	2.8
1	B	385	SER	2.8
1	C	198	PRO	2.8
1	A	250	MET	2.8
1	D	399	HIS	2.8
1	B	232	GLU	2.7
1	C	257	VAL	2.7
1	D	383	GLY	2.7
1	B	352	TRP	2.4
1	B	387	LEU	2.4
1	A	338	ARG	2.4
1	C	383	GLY	2.3
1	A	424	PRO	2.3
1	A	253	THR	2.3
1	D	387	LEU	2.2
1	D	314	ASP	2.2
1	D	375	LEU	2.2
1	D	194	ARG	2.1
1	C	314	ASP	2.1
1	B	255	ARG	2.1
1	C	251	SER	2.1
1	A	399	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	399	HIS	2.1
1	B	384	ALA	2.0
1	D	251	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	SEP	D	386	10/11	0.71	0.23	-	58,62,63,64	0
1	SEP	C	386	10/11	0.47	0.30	-	51,56,63,64	0
1	SEP	B	386	10/11	0.80	0.21	-	54,56,61,62	0
1	SEP	A	386	10/11	0.98	0.07	-	11,13,15,15	0
1	SEP	D	402	10/11	0.67	0.22	-	33,39,50,50	0
1	SEP	A	402	10/11	0.90	0.12	-	16,20,31,31	0
1	SEP	C	402	10/11	0.76	0.17	-	26,32,45,45	0
1	SEP	B	402	10/11	0.74	0.21	-	32,39,49,49	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, 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
3	MPD	B	3001	8/8	0.69	0.31	20.34	59,59,60,61	0
3	MPD	A	3002	8/8	0.63	0.33	14.83	53,55,55,55	0
3	MPD	C	3003	8/8	0.59	0.34	13.49	59,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MPD	D	3004	8/8	0.74	0.22	5.52	58,59,59,59	0
2	ACY	C	2003	4/4	0.84	0.15	3.39	29,33,35,35	0
2	ACY	A	2001	4/4	0.72	0.22	2.73	35,38,38,40	0

6.5 Other polymers (i)

There are no such residues in this entry.