Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 08:47 AM EDT

PDB ID	:	3NK4
Title	:	Crystal structure of full-length sperm receptor ZP3 at 2.0 A resolution
Authors	:	Monne, M.; Jovine, L.
Deposited on	:	2010-06-18
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

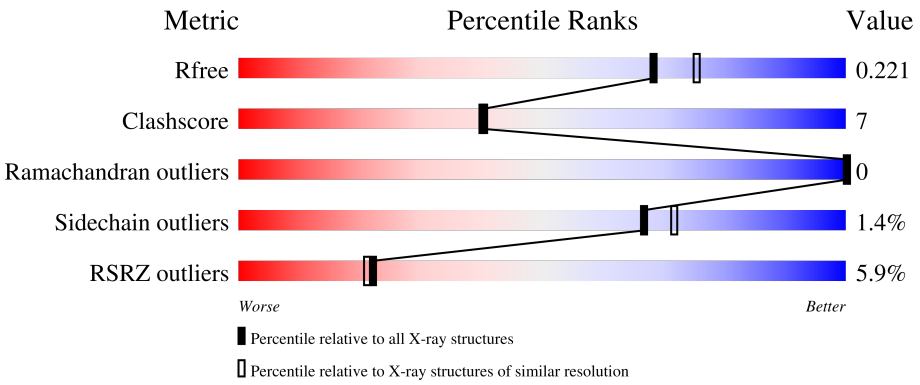
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	297	4% 79% 14% 7%
1	B	297	6% 76% 14% 10%
2	C	30	10% 50% 23% 27%
2	D	30	3% 33% 13% 53%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9074 atoms, of which 4347 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 Zona pellucida 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	277	4205	1344	2061	379	408	13	0	0	0
1	B	268	4077	1295	2004	369	396	13	0	2	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P79762
A	?	-	TRP	deletion	UNP P79762
A	?	-	ASP	deletion	UNP P79762
A	?	-	ILE	deletion	UNP P79762
A	?	-	SER	deletion	UNP P79762
A	?	-	TRP	deletion	UNP P79762
A	?	-	ALA	deletion	UNP P79762
A	?	-	ALA	deletion	UNP P79762
A	?	-	ARG	deletion	UNP P79762
A	?	-	GLY	deletion	UNP P79762
A	?	-	ASP	deletion	UNP P79762
A	?	-	PRO	deletion	UNP P79762
A	?	-	SER	deletion	UNP P79762
A	?	-	ALA	deletion	UNP P79762
A	?	-	TRP	deletion	UNP P79762
A	?	-	SER	deletion	UNP P79762
A	?	-	TRP	deletion	UNP P79762
A	?	-	GLY	deletion	UNP P79762
A	?	-	ALA	deletion	UNP P79762
A	?	-	GLU	deletion	UNP P79762
A	?	-	ALA	deletion	UNP P79762
A	?	-	HIS	deletion	UNP P79762
A	?	-	SER	deletion	UNP P79762
A	?	-	ARG	deletion	UNP P79762
A	?	-	ALA	deletion	UNP P79762

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P79762
A	?	-	ALA	deletion	UNP P79762
A	?	-	GLY	deletion	UNP P79762
A	?	-	SER	deletion	UNP P79762
A	?	-	HIS	deletion	UNP P79762
A	159	GLN	ASN	engineered mutation	UNP P79762
B	?	-	PRO	deletion	UNP P79762
B	?	-	TRP	deletion	UNP P79762
B	?	-	ASP	deletion	UNP P79762
B	?	-	ILE	deletion	UNP P79762
B	?	-	SER	deletion	UNP P79762
B	?	-	TRP	deletion	UNP P79762
B	?	-	ALA	deletion	UNP P79762
B	?	-	ALA	deletion	UNP P79762
B	?	-	ARG	deletion	UNP P79762
B	?	-	GLY	deletion	UNP P79762
B	?	-	ASP	deletion	UNP P79762
B	?	-	PRO	deletion	UNP P79762
B	?	-	SER	deletion	UNP P79762
B	?	-	ALA	deletion	UNP P79762
B	?	-	TRP	deletion	UNP P79762
B	?	-	SER	deletion	UNP P79762
B	?	-	TRP	deletion	UNP P79762
B	?	-	GLY	deletion	UNP P79762
B	?	-	ALA	deletion	UNP P79762
B	?	-	GLU	deletion	UNP P79762
B	?	-	ALA	deletion	UNP P79762
B	?	-	HIS	deletion	UNP P79762
B	?	-	SER	deletion	UNP P79762
B	?	-	ARG	deletion	UNP P79762
B	?	-	ALA	deletion	UNP P79762
B	?	-	VAL	deletion	UNP P79762
B	?	-	ALA	deletion	UNP P79762
B	?	-	GLY	deletion	UNP P79762
B	?	-	SER	deletion	UNP P79762
B	?	-	HIS	deletion	UNP P79762
B	159	GLN	ASN	engineered mutation	UNP P79762

- Molecule 2 is a protein called Zona pellucida 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	22	325	106	155	34	30	0	0	0

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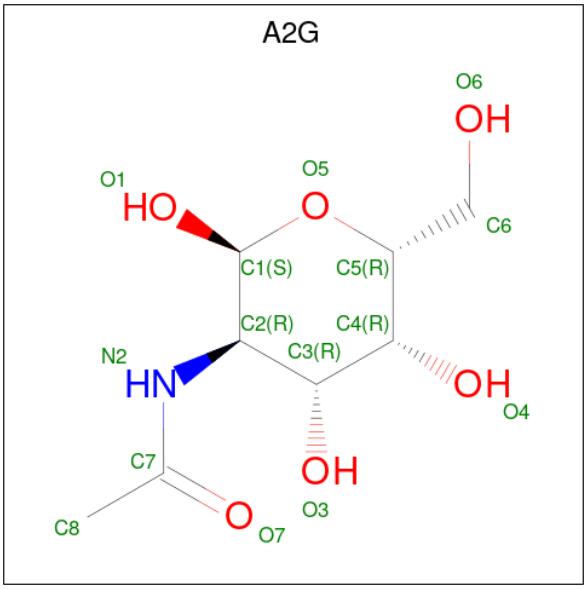
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	D	14	195	61	103	14	17	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

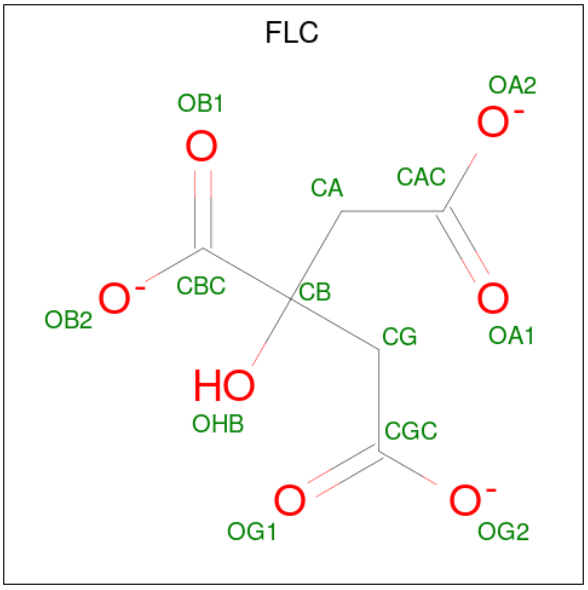
Chain	Residue	Modelled	Actual	Comment	Reference
C	359	ALA	ARG	engineered mutation	UNP P79762
C	361	ALA	ARG	engineered mutation	UNP P79762
C	362	ALA	ARG	engineered mutation	UNP P79762
C	383	HIS	-	expression tag	UNP P79762
C	384	HIS	-	expression tag	UNP P79762
C	385	HIS	-	expression tag	UNP P79762
C	386	HIS	-	expression tag	UNP P79762
C	387	HIS	-	expression tag	UNP P79762
C	388	HIS	-	expression tag	UNP P79762
D	359	ALA	ARG	engineered mutation	UNP P79762
D	361	ALA	ARG	engineered mutation	UNP P79762
D	362	ALA	ARG	engineered mutation	UNP P79762
D	383	HIS	-	expression tag	UNP P79762
D	384	HIS	-	expression tag	UNP P79762
D	385	HIS	-	expression tag	UNP P79762
D	386	HIS	-	expression tag	UNP P79762
D	387	HIS	-	expression tag	UNP P79762
D	388	HIS	-	expression tag	UNP P79762

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	28	8	14	1	5	0	0

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	18	6	5	7	0	0
			Total	C	H	O		
4	C	1	18	6	5	7	0	0

- Molecule 5 is water.

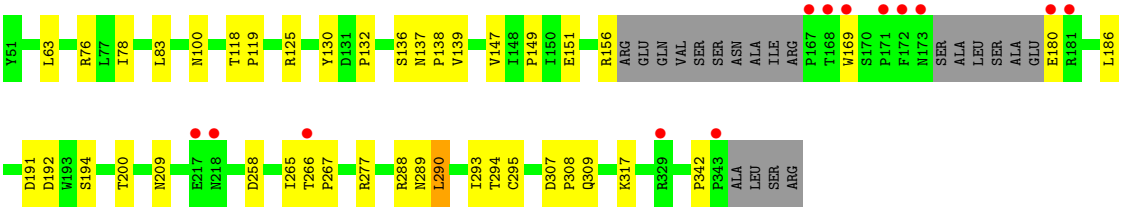
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	101	101	101	0	0
			Total	O		
5	B	84	84	84	0	0
			Total	O		
5	C	15	15	15	0	0
			Total	O		
5	D	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

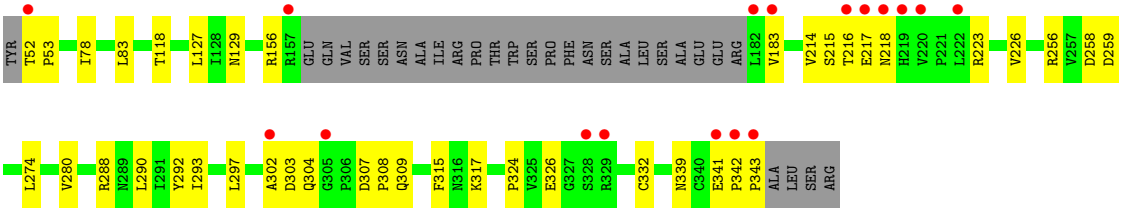
• Molecule 1: Zona pellucida 3

Chain A:



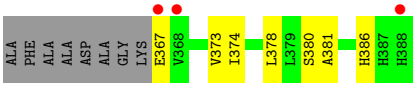
• Molecule 1: Zona pellucida 3

Chain B:



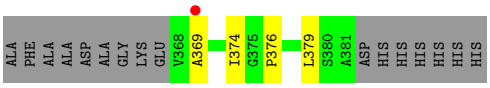
• Molecule 2: Zona pellucida 3

Chain C:



• Molecule 2: Zona pellucida 3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.70Å 97.70Å 256.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.34 – 2.00 36.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.34-2.00) 99.9 (36.34-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.208 , 0.226 0.203 , 0.221	Depositor DCC
R_{free} test set	4213 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9074	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A2G, FLC

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	0.46	0/2197	0.60	0/3005
1	B	0.50	0/2127	0.61	0/2910
2	C	0.47	0/176	0.53	0/240
2	D	0.41	0/92	0.67	0/127
All	All	0.48	0/4592	0.61	0/6282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2144	2061	2059	29	0
1	B	2073	2004	2004	31	0
2	C	170	155	154	6	0
2	D	92	103	102	4	0
3	A	14	14	12	0	0
4	A	13	5	5	2	0
4	C	13	5	5	2	0
5	A	101	0	0	2	0
5	B	84	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	15	0	0	1	0
5	D	8	0	0	0	0
All	All	4727	4347	4341	64	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 7.

All (64) 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:A:191:ASP:HA	1:A:209:ASN:ND2	2.05	0.71
1:B:183:VAL:CG2	1:B:215:SER:HB3	2.26	0.66
1:A:78:ILE:HD11	1:A:83:LEU:HD11	1.78	0.64
1:B:216:THR:HG22	1:B:216:THR:O	1.99	0.63
1:B:183:VAL:HG22	1:B:215:SER:HB3	1.81	0.62
1:A:125:ARG:HG2	1:A:151:GLU:HG3	1.86	0.58
1:B:307:ASP:HB2	1:B:308:PRO:CD	2.33	0.58
1:A:191:ASP:HA	1:A:209:ASN:HD21	1.67	0.58
1:B:78:ILE:HD11	1:B:83:LEU:HD11	1.85	0.57
1:B:258:ASP:O	1:B:317:LYS:HE2	2.06	0.56
1:A:288:ARG:O	1:A:289:ASN:HB2	2.07	0.55
1:B:226:VAL:HG22	1:B:297:LEU:HD22	1.87	0.55
1:B:129[B]:ASN:ND2	1:B:288:ARG:HD2	2.23	0.54
1:A:307:ASP:HB2	1:A:308:PRO:CD	2.38	0.54
1:B:183:VAL:HG22	1:B:215:SER:CB	2.37	0.54
1:A:265:ILE:HD11	1:A:277:ARG:CD	2.39	0.53
1:A:289:ASN:HA	5:A:30:HOH:O	2.09	0.53
1:B:324:PRO:HG3	1:B:332:CYS:SG	2.50	0.52
1:A:266:THR:CG2	1:A:267:PRO:HA	2.39	0.52
1:A:258:ASP:O	1:A:317:LYS:HE2	2.09	0.51
1:A:100:ASN:ND2	5:A:422:HOH:O	2.43	0.51
1:B:52:THR:OG1	1:B:53:PRO:N	2.41	0.51
1:B:293:ILE:HB	2:D:374:ILE:HG22	1.93	0.51
1:B:118:THR:O	1:B:156:ARG:HD2	2.12	0.50
1:B:307:ASP:HB2	1:B:308:PRO:HD2	1.93	0.50
1:A:290:LEU:HD12	1:A:290:LEU:O	2.12	0.50
1:B:309:GLN:OE1	1:B:342:PRO:HD3	2.13	0.49
2:C:386:HIS:HD1	4:C:910:FLC:CBC	2.24	0.49
1:A:169:TRP:CG	1:A:180:GLU:HG2	2.48	0.49
1:B:256:ARG:HD2	1:B:315:PHE:CD2	2.48	0.48
1:B:127:LEU:C	1:B:127:LEU:HD12	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:HB2	1:A:308:PRO:HD2	1.96	0.48
1:A:136:SER:O	1:A:138:PRO:HD3	2.14	0.47
4:A:911:FLC:OA1	4:A:911:FLC:OB1	2.33	0.47
4:A:911:FLC:CGC	4:A:911:FLC:OB2	2.63	0.46
1:B:339:ASN:OD1	1:B:339:ASN:C	2.54	0.46
1:A:137:ASN:OD1	1:A:139:VAL:HG22	2.16	0.46
1:B:226:VAL:HG23	1:B:274:LEU:HD23	1.98	0.45
1:A:265:ILE:HD11	1:A:277:ARG:HD2	1.97	0.45
1:B:223:ARG:NH1	1:B:302:ALA:O	2.49	0.45
1:A:63:LEU:C	1:A:63:LEU:HD12	2.36	0.45
1:A:192:ASP:OD2	1:A:194:SER:HB3	2.17	0.45
1:A:76:ARG:HD2	1:B:259:ASP:OD2	2.17	0.44
1:B:290:LEU:C	1:B:290:LEU:HD12	2.38	0.44
1:A:130:TYR:CE2	1:A:132:PRO:HG3	2.53	0.44
1:B:297:LEU:O	2:D:369:ALA:HB1	2.18	0.44
4:C:910:FLC:CBC	4:C:910:FLC:OG2	2.67	0.43
1:A:293:ILE:HB	2:C:374:ILE:CG2	2.47	0.43
1:B:292:TYR:CZ	2:D:376:PRO:HB3	2.54	0.43
1:A:290:LEU:HD12	1:A:290:LEU:C	2.38	0.43
2:C:381:ALA:O	5:C:182:HOH:O	2.21	0.43
1:B:127:LEU:HD12	1:B:127:LEU:O	2.19	0.43
1:A:200:THR:HG22	2:C:378:LEU:HD12	2.01	0.42
1:B:218:ASN:N	1:B:218:ASN:OD1	2.52	0.42
1:B:303:ASP:OD1	1:B:304:GLN:N	2.52	0.42
1:B:341:GLU:O	1:B:343:PRO:HD3	2.19	0.42
1:A:294:THR:HB	2:C:373:VAL:HG22	2.02	0.42
1:B:256:ARG:HD2	1:B:315:PHE:CE2	2.55	0.42
1:A:309:GLN:OE1	1:A:342:PRO:HG3	2.20	0.41
1:A:149:PRO:HG3	2:C:378:LEU:CD1	2.50	0.41
1:A:186:LEU:HD11	1:A:295:CYS:HB2	2.02	0.41
1:A:118:THR:HB	1:A:119:PRO:CD	2.50	0.41
1:B:280:VAL:CG1	2:D:379:LEU:HD21	2.51	0.40
1:B:214:VAL:O	1:B:214:VAL:HG13	2.21	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	271/297 (91%)	264 (97%)	7 (3%)	0	100	100
1	B	266/297 (90%)	257 (97%)	9 (3%)	0	100	100
2	C	20/30 (67%)	20 (100%)	0	0	100	100
2	D	12/30 (40%)	12 (100%)	0	0	100	100
All	All	569/654 (87%)	553 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	242/258 (94%)	239 (99%)	3 (1%)	71	76
1	B	235/258 (91%)	233 (99%)	2 (1%)	78	83
2	C	18/21 (86%)	16 (89%)	2 (11%)	6	3
2	D	10/21 (48%)	10 (100%)	0	100	100
All	All	505/558 (90%)	498 (99%)	7 (1%)	67	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	VAL
1	A	156	ARG

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Mol	Chain	Res	Type
1	A	290	LEU
1	B	217	GLU
1	B	326	GLU
2	C	367	GLU
2	C	380	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	310	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	A2G	A	900	1	14,14,15	0.66	0	17,19,21	1.22	3 (17%)
4	FLC	C	910	-	12,12,12	2.13	1 (8%)	17,17,17	2.33	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FLC	A	911	-	12,12,12	0.92	0	17,17,17	1.35	2 (11%)

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	A2G	A	900	1	-	0/6/23/26	0/1/1/1
4	FLC	C	910	-	-	3/16/16/16	-
4	FLC	A	911	-	-	4/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	910	FLC	CB-CBC	-6.57	1.46	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	910	FLC	OB1-CBC-CB	-4.85	115.38	122.25
4	C	910	FLC	OHB-CB-CBC	-4.27	102.87	108.86
4	A	911	FLC	OB2-CBC-CB	3.70	119.47	113.05
4	C	910	FLC	OHB-CB-CA	2.87	116.11	109.40
4	C	910	FLC	CA-CB-CBC	-2.71	104.28	110.11
4	C	910	FLC	OA2-CAC-CA	2.71	123.04	114.35
4	C	910	FLC	OG2-CGC-CG	2.35	121.89	114.35
3	A	900	A2G	O7-C7-N2	2.30	126.19	121.95
3	A	900	A2G	C3-C4-C5	-2.22	106.27	110.24
3	A	900	A2G	C8-C7-N2	-2.12	112.51	116.10
4	C	910	FLC	OG1-CGC-CG	-2.10	116.80	122.94
4	A	911	FLC	OG1-CGC-CG	-2.03	117.02	122.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	911	FLC	CA-CB-CBC-OB1
4	A	911	FLC	CA-CB-CBC-OB2
4	A	911	FLC	OHB-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
4	A	911	FLC	OHB-CB-CBC-OB2
4	C	910	FLC	CAC-CA-CB-CBC
4	C	910	FLC	CAC-CA-CB-CG
4	C	910	FLC	CAC-CA-CB-OHB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	910	FLC	2	0
4	A	911	FLC	2	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	277/297 (93%)	0.16	13 (4%)	31	30	39, 61, 107, 166	0
1	B	268/297 (90%)	0.20	17 (6%)	20	19	40, 65, 127, 174	0
2	C	22/30 (73%)	0.45	3 (13%)	3	2	50, 59, 85, 140	0
2	D	14/30 (46%)	0.48	1 (7%)	16	15	52, 64, 98, 112	0
All	All	581/654 (88%)	0.20	34 (5%)	22	21	39, 63, 122, 174	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	PRO	7.0
1	B	343	PRO	5.8
1	A	180	GLU	5.6
1	A	169	TRP	5.5
1	B	216	THR	5.5
1	B	218	ASN	5.3
1	B	219	HIS	5.1
1	A	172	PHE	5.1
1	A	173	ASN	4.9
1	A	167	PRO	4.7
1	B	157	ARG	4.4
1	A	181	ARG	4.3
1	B	220	VAL	4.2
1	B	217	GLU	3.8
1	B	302	ALA	3.7
1	A	217	GLU	3.6
2	C	388	HIS	3.5
2	C	367	GLU	3.5
1	B	342	PRO	3.3
1	A	168	THR	3.1
1	B	52	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	183	VAL	2.8
1	A	329	ARG	2.7
1	A	171	PRO	2.7
2	D	369	ALA	2.6
1	B	182	LEU	2.6
1	A	218	ASN	2.4
1	A	266	THR	2.3
1	B	341	GLU	2.3
1	B	328	SER	2.3
1	B	222	LEU	2.2
1	B	305	GLY	2.1
2	C	368	VAL	2.1
1	B	329	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	FLC	A	911	13/13	0.76	0.33	103,123,138,148	0
3	A2G	A	900	14/15	0.84	0.39	133,181,211,217	0
4	FLC	C	910	13/13	0.93	0.13	51,75,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.