Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 10:43 PM EDT

PDB ID	:	6ND8
Title	:	RHODOCETIN IN COMPLEX WITH THE INTEGRIN ALPHA2-A DOMAIN AND BARIUM
Authors	:	Stetefeld, J.; McDougall, M.D.; Loewen, P.C.
Deposited on	:	2018-12-13
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
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:

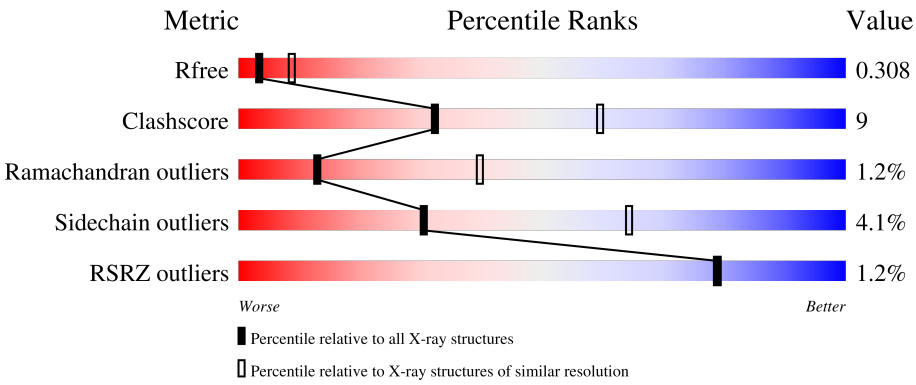
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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	135	73% 23% • •
1	D	135	73% 21% • •
1	G	135	77% 16% • •
1	J	135	81% 15% • •
1	M	135	3% 65% 29% • •

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Mol	Chain	Length	Quality of chain
1	P	135	2%, 64%, 32%
2	B	124	2%, 77%, 20%
2	E	124	68%, 28%
2	H	124	72%, 27%
2	K	124	2%, 72%, 23%
2	N	124	3%, 72%, 24%
2	Q	124	5%, 73%, 21%
3	C	217	71%, 17%, 12%
3	F	217	%, 68%, 20%, 12%
3	I	217	%, 70%, 17%, 12%
3	L	217	%, 71%, 16%, 12%
3	O	217	73%, 15%, 12%
3	R	217	76%, 12%, 12%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21590 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 Snaclec rhodocetin subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	131	1070	672	189	200	9	0	0	0
1	D	131	1070	672	189	200	9	0	0	0
1	G	131	1070	672	189	200	9	0	0	0
1	J	131	1070	672	189	200	9	0	0	0
1	M	131	1070	672	189	200	9	0	0	0
1	P	131	1070	672	189	200	9	0	0	0

- Molecule 2 is a protein called Snaclec rhodocetin subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	122	1029	667	174	179	9	0	0	0
2	E	122	1029	667	174	179	9	0	0	0
2	H	122	1029	667	174	179	9	0	0	0
2	K	122	1029	667	174	179	9	0	0	0
2	N	122	1029	667	174	179	9	0	0	0
2	Q	122	1029	667	174	179	9	0	0	0

- Molecule 3 is a protein called Integrin alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	191	1482	940	250	287	5	0	0	0
3	F	191	1482	940	250	287	5	0	0	0
3	I	191	1482	940	250	287	5	0	0	0
3	L	191	1482	940	250	287	5	0	0	0
3	O	191	1482	940	250	287	5	0	0	0
3	R	191	1482	940	250	287	5	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	MET	-	expression tag	UNP P17301
C	151	GLY	-	expression tag	UNP P17301
C	152	SER	-	expression tag	UNP P17301
C	153	SER	-	expression tag	UNP P17301
C	154	HIS	-	expression tag	UNP P17301
C	155	HIS	-	expression tag	UNP P17301
C	156	HIS	-	expression tag	UNP P17301
C	157	HIS	-	expression tag	UNP P17301
C	158	HIS	-	expression tag	UNP P17301
C	159	HIS	-	expression tag	UNP P17301
C	160	SER	-	expression tag	UNP P17301
C	161	SER	-	expression tag	UNP P17301
C	162	GLY	-	expression tag	UNP P17301
C	163	LEU	-	expression tag	UNP P17301
C	164	VAL	-	expression tag	UNP P17301
C	165	PRO	-	expression tag	UNP P17301
C	166	ARG	-	expression tag	UNP P17301
C	167	GLY	-	expression tag	UNP P17301
C	168	GLY	-	expression tag	UNP P17301
C	169	SER	-	expression tag	UNP P17301
F	150	MET	-	expression tag	UNP P17301
F	151	GLY	-	expression tag	UNP P17301
F	152	SER	-	expression tag	UNP P17301
F	153	SER	-	expression tag	UNP P17301
F	154	HIS	-	expression tag	UNP P17301
F	155	HIS	-	expression tag	UNP P17301
F	156	HIS	-	expression tag	UNP P17301
F	157	HIS	-	expression tag	UNP P17301

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Chain	Residue	Modelled	Actual	Comment	Reference
F	158	HIS	-	expression tag	UNP P17301
F	159	HIS	-	expression tag	UNP P17301
F	160	SER	-	expression tag	UNP P17301
F	161	SER	-	expression tag	UNP P17301
F	162	GLY	-	expression tag	UNP P17301
F	163	LEU	-	expression tag	UNP P17301
F	164	VAL	-	expression tag	UNP P17301
F	165	PRO	-	expression tag	UNP P17301
F	166	ARG	-	expression tag	UNP P17301
F	167	GLY	-	expression tag	UNP P17301
F	168	GLY	-	expression tag	UNP P17301
F	169	SER	-	expression tag	UNP P17301
I	150	MET	-	expression tag	UNP P17301
I	151	GLY	-	expression tag	UNP P17301
I	152	SER	-	expression tag	UNP P17301
I	153	SER	-	expression tag	UNP P17301
I	154	HIS	-	expression tag	UNP P17301
I	155	HIS	-	expression tag	UNP P17301
I	156	HIS	-	expression tag	UNP P17301
I	157	HIS	-	expression tag	UNP P17301
I	158	HIS	-	expression tag	UNP P17301
I	159	HIS	-	expression tag	UNP P17301
I	160	SER	-	expression tag	UNP P17301
I	161	SER	-	expression tag	UNP P17301
I	162	GLY	-	expression tag	UNP P17301
I	163	LEU	-	expression tag	UNP P17301
I	164	VAL	-	expression tag	UNP P17301
I	165	PRO	-	expression tag	UNP P17301
I	166	ARG	-	expression tag	UNP P17301
I	167	GLY	-	expression tag	UNP P17301
I	168	GLY	-	expression tag	UNP P17301
I	169	SER	-	expression tag	UNP P17301
L	150	MET	-	expression tag	UNP P17301
L	151	GLY	-	expression tag	UNP P17301
L	152	SER	-	expression tag	UNP P17301
L	153	SER	-	expression tag	UNP P17301
L	154	HIS	-	expression tag	UNP P17301
L	155	HIS	-	expression tag	UNP P17301
L	156	HIS	-	expression tag	UNP P17301
L	157	HIS	-	expression tag	UNP P17301
L	158	HIS	-	expression tag	UNP P17301
L	159	HIS	-	expression tag	UNP P17301

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Chain	Residue	Modelled	Actual	Comment	Reference
L	160	SER	-	expression tag	UNP P17301
L	161	SER	-	expression tag	UNP P17301
L	162	GLY	-	expression tag	UNP P17301
L	163	LEU	-	expression tag	UNP P17301
L	164	VAL	-	expression tag	UNP P17301
L	165	PRO	-	expression tag	UNP P17301
L	166	ARG	-	expression tag	UNP P17301
L	167	GLY	-	expression tag	UNP P17301
L	168	GLY	-	expression tag	UNP P17301
L	169	SER	-	expression tag	UNP P17301
O	150	MET	-	expression tag	UNP P17301
O	151	GLY	-	expression tag	UNP P17301
O	152	SER	-	expression tag	UNP P17301
O	153	SER	-	expression tag	UNP P17301
O	154	HIS	-	expression tag	UNP P17301
O	155	HIS	-	expression tag	UNP P17301
O	156	HIS	-	expression tag	UNP P17301
O	157	HIS	-	expression tag	UNP P17301
O	158	HIS	-	expression tag	UNP P17301
O	159	HIS	-	expression tag	UNP P17301
O	160	SER	-	expression tag	UNP P17301
O	161	SER	-	expression tag	UNP P17301
O	162	GLY	-	expression tag	UNP P17301
O	163	LEU	-	expression tag	UNP P17301
O	164	VAL	-	expression tag	UNP P17301
O	165	PRO	-	expression tag	UNP P17301
O	166	ARG	-	expression tag	UNP P17301
O	167	GLY	-	expression tag	UNP P17301
O	168	GLY	-	expression tag	UNP P17301
O	169	SER	-	expression tag	UNP P17301
R	150	MET	-	expression tag	UNP P17301
R	151	GLY	-	expression tag	UNP P17301
R	152	SER	-	expression tag	UNP P17301
R	153	SER	-	expression tag	UNP P17301
R	154	HIS	-	expression tag	UNP P17301
R	155	HIS	-	expression tag	UNP P17301
R	156	HIS	-	expression tag	UNP P17301
R	157	HIS	-	expression tag	UNP P17301
R	158	HIS	-	expression tag	UNP P17301
R	159	HIS	-	expression tag	UNP P17301
R	160	SER	-	expression tag	UNP P17301
R	161	SER	-	expression tag	UNP P17301

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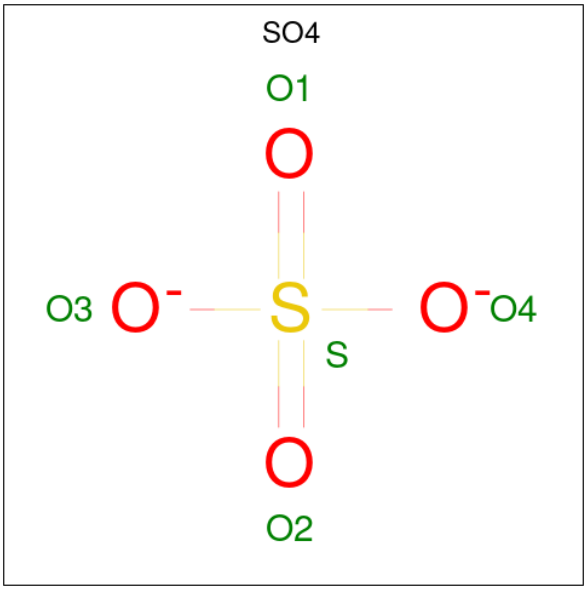
Chain	Residue	Modelled	Actual	Comment	Reference
R	162	GLY	-	expression tag	UNP P17301
R	163	LEU	-	expression tag	UNP P17301
R	164	VAL	-	expression tag	UNP P17301
R	165	PRO	-	expression tag	UNP P17301
R	166	ARG	-	expression tag	UNP P17301
R	167	GLY	-	expression tag	UNP P17301
R	168	GLY	-	expression tag	UNP P17301
R	169	SER	-	expression tag	UNP P17301

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	O	1	Total O S 5 4 1	0	0
4	Q	1	Total O S 5 4 1	0	0
4	Q	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0

- Molecule 5 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Ba 1 1	0	0
5	F	1	Total Ba 1 1	0	0
5	I	1	Total Ba 1 1	0	0
5	L	1	Total Ba 1 1	0	0
5	O	1	Total Ba 1 1	0	0
5	R	1	Total Ba 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Na 1 1	0	0
6	F	1	Total Na 1 1	0	0
6	I	1	Total Na 1 1	0	0

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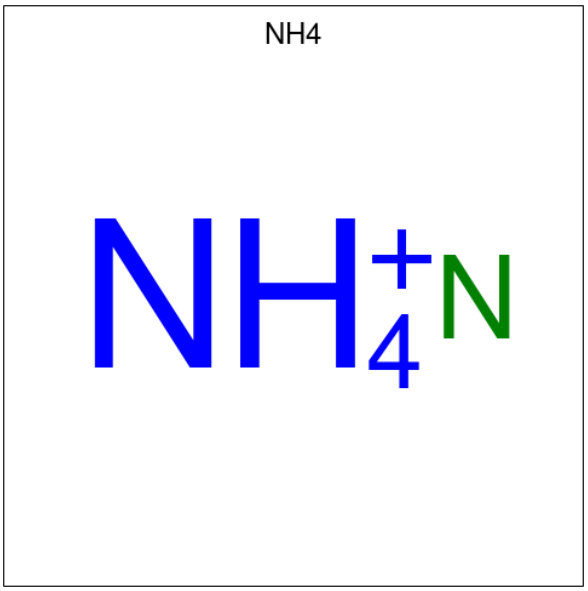
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	L	1	1	1	0	0
			Total	Na		
6	O	1	1	1	0	0
			Total	Na		
6	R	1	1	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	C	2	2	2	0	0
			Total	Cl		
7	E	1	1	1	0	0
			Total	Cl		
7	H	1	1	1	0	0
			Total	Cl		
7	J	1	1	1	0	0
			Total	Cl		
7	K	1	1	1	0	0
			Total	Cl		
7	L	1	1	1	0	0
			Total	Cl		
7	M	1	1	1	0	0
			Total	Cl		
7	R	1	1	1	0	0

- Molecule 8 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total N 1 1	0	0

- Molecule 9 is water.

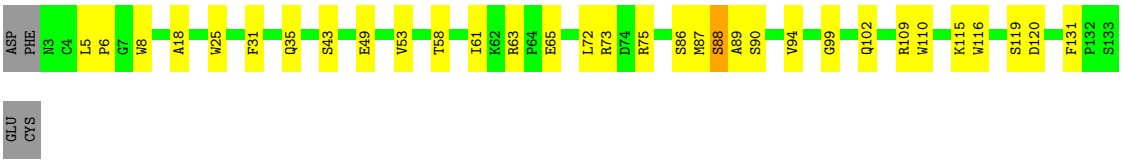
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	5	Total O 5 5	0	0
9	D	1	Total O 1 1	0	0
9	F	1	Total O 1 1	0	0

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.

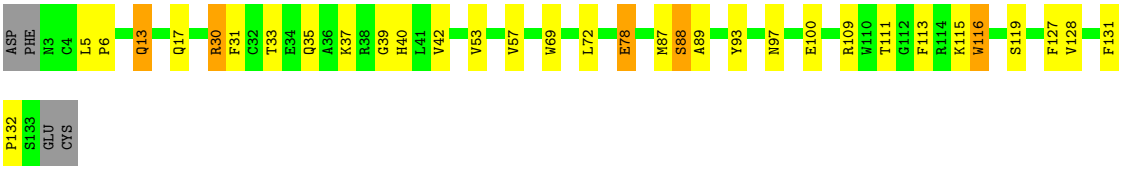
• Molecule 1: Snaclec rhodocetin subunit gamma

Chain A: 73% 23%



• Molecule 1: Snaclec rhodocetin subunit gamma

Chain D: 73% 21%



• Molecule 1: Snaclec rhodocetin subunit gamma

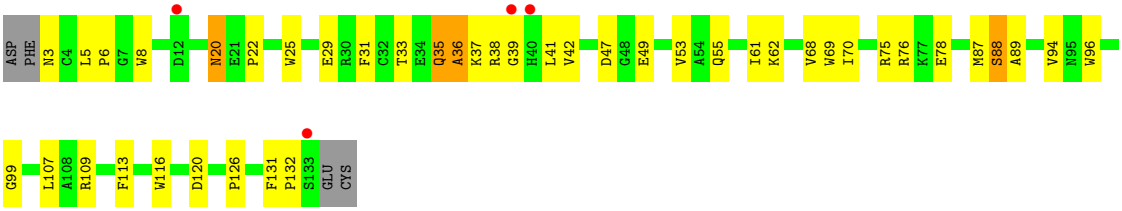
Chain G: 77% 16%

• Molecule 1: Snaclec rhodocetin subunit gamma

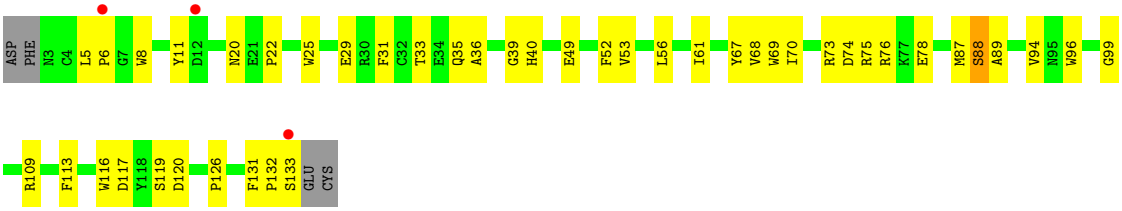
Chain J: 81% 15%

• Molecule 1: Snaclec rhodocetin subunit gamma

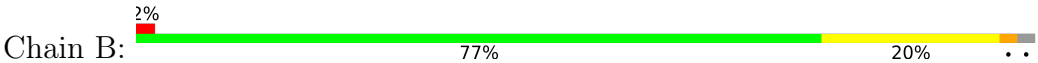
Chain M: 3% 65% 29%

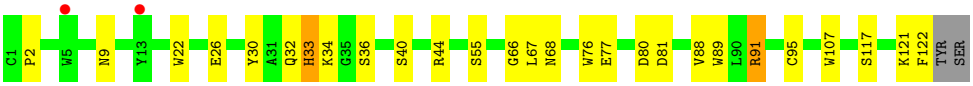


• Molecule 1: Snaclec rhodocetin subunit gamma



• Molecule 2: Snaclec rhodocetin subunit delta





• Molecule 2: Snaclec rhodocetin subunit delta

• Molecule 2: Snaclec rhodocetin subunit delta

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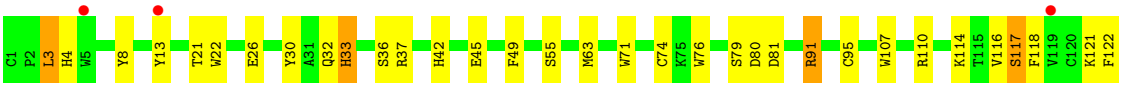
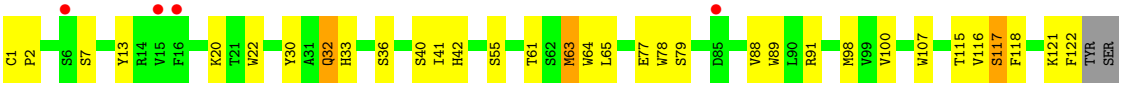


TYR SER

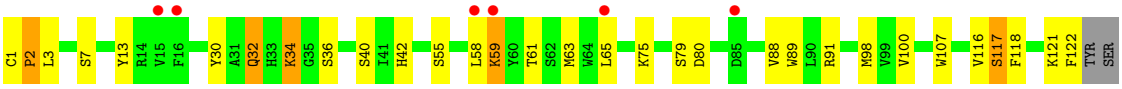
• Molecule 2: Snaclec rhodocetin subunit delta

Chain N:



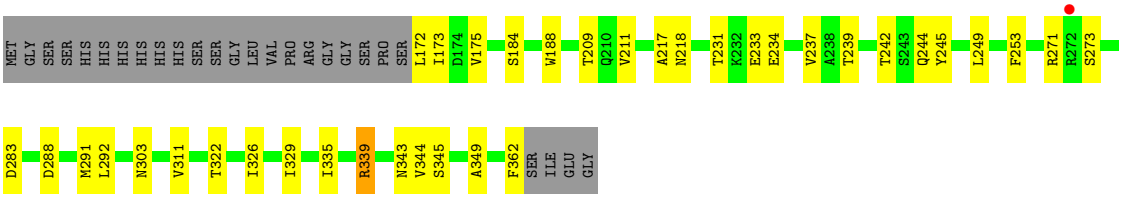
• Molecule 2: Snaclec rhodocetin subunit delta

Chain Q:



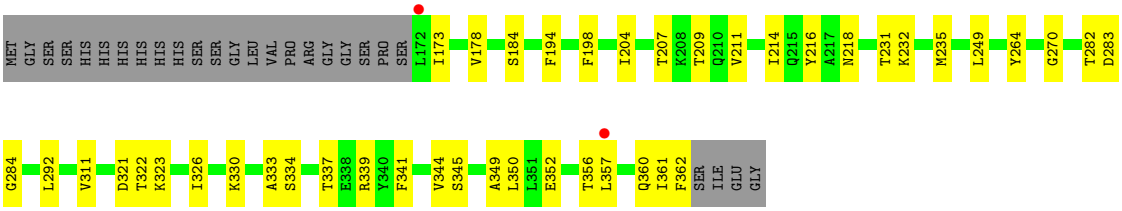
• Molecule 3: Integrin alpha-2

Chain C:



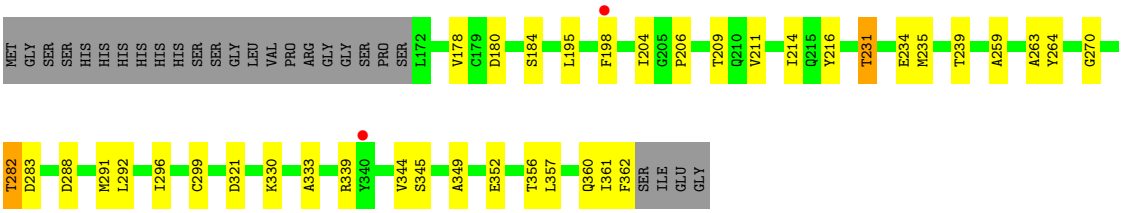
• Molecule 3: Integrin alpha-2

Chain F:



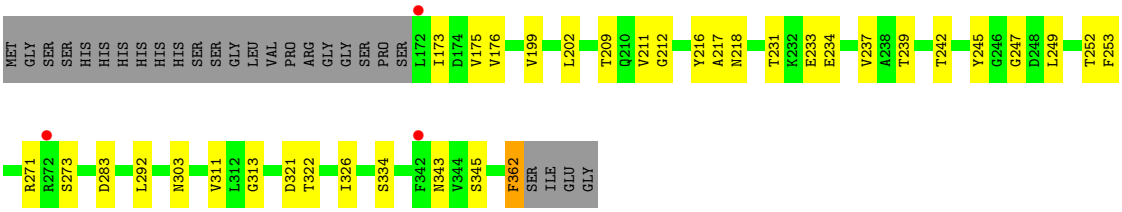
• Molecule 3: Integrin alpha-2

Chain I:



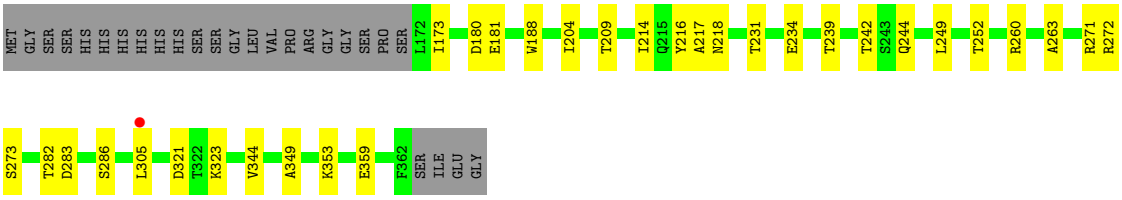
• Molecule 3: Integrin alpha-2

Chain L:



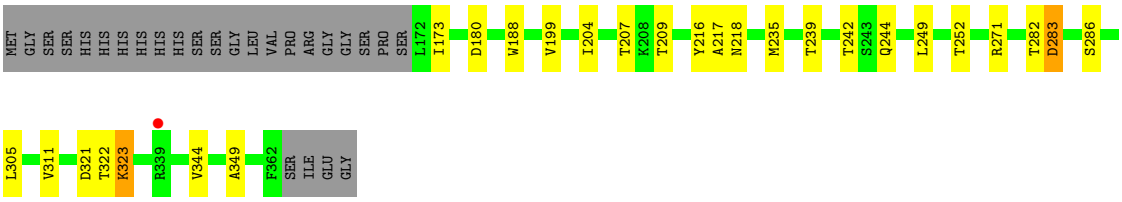
- Molecule 3: Integrin alpha-2

Chain O:



- Molecule 3: Integrin alpha-2

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	131.13Å 131.13Å 251.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.90 45.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.64-2.90) 97.9 (45.59-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.247 , 0.306 0.250 , 0.308	Depositor DCC
R_{free} test set	4494 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 15.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	21590	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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, 0.333 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: NA, NH4, SO4, CL, BA

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	0.69	0/1101	0.80	0/1491
1	D	0.69	0/1101	0.81	0/1491
1	G	0.69	0/1101	0.81	0/1491
1	J	0.68	0/1101	0.81	0/1491
1	M	0.70	0/1101	0.83	0/1491
1	P	0.71	0/1101	0.82	0/1491
2	B	0.68	0/1064	0.83	0/1439
2	E	0.67	0/1064	0.79	0/1439
2	H	0.66	0/1064	0.80	0/1439
2	K	0.67	0/1064	0.81	0/1439
2	N	0.68	0/1064	0.82	0/1439
2	Q	0.68	0/1064	0.83	0/1439
3	C	0.69	0/1506	0.79	0/2040
3	F	0.69	0/1506	0.84	1/2040 (0.0%)
3	I	0.70	0/1506	0.82	0/2040
3	L	0.70	0/1506	0.80	0/2040
3	O	0.70	0/1506	0.80	0/2040
3	R	0.70	0/1506	0.81	0/2040
All	All	0.69	0/22026	0.81	1/29820 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	323	LYS	CB-CA-C	5.16	120.72	110.40

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	1070	0	988	30	0
1	D	1070	0	988	22	0
1	G	1070	0	988	22	0
1	J	1070	0	988	20	0
1	M	1070	0	988	40	0
1	P	1070	0	988	36	0
2	B	1029	0	977	22	0
2	E	1029	0	977	29	0
2	H	1029	0	977	28	0
2	K	1029	0	977	22	0
2	N	1029	0	977	28	0
2	Q	1029	0	977	27	0
3	C	1482	0	1477	18	0
3	F	1482	0	1477	23	0
3	I	1482	0	1477	20	0
3	L	1482	0	1477	19	0
3	O	1482	0	1477	18	0
3	R	1482	0	1478	17	0
4	A	10	0	0	1	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	J	5	0	0	0	0
4	K	5	0	0	0	0
4	N	5	0	0	0	0
4	O	5	0	0	1	0
4	Q	10	0	0	0	0
4	R	5	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
5	O	1	0	0	0	0
5	R	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	L	1	0	0	0	0
6	O	1	0	0	0	0
6	R	1	0	0	0	0
7	C	2	0	0	1	0
7	E	1	0	0	0	0
7	H	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	R	1	0	0	0	0
8	D	1	0	0	1	0
9	A	5	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
All	All	21590	0	20653	373	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 (373) 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:P:87:MET:SD	2:Q:40:SER:OG	2.30	0.89
1:P:29:GLU:OE2	2:Q:79:SER:OG	1.90	0.88
1:M:29:GLU:OE2	2:N:79:SER:OG	1.93	0.86
1:M:87:MET:SD	2:N:40:SER:OG	2.34	0.86
2:E:14:ARG:NH1	3:O:359:GLU:OE2	2.09	0.84
2:E:31:ALA:HB1	3:O:353:LYS:HE2	1.63	0.81
1:D:17:GLN:OE1	8:D:202:NH4:N	2.14	0.81
3:R:204:ILE:HG12	3:R:235:MET:HE1	1.61	0.80
1:A:43:SER:HB3	2:B:80:ASP:OD2	1.84	0.78
1:P:89:ALA:HB1	2:Q:42:HIS:CE1	2.23	0.73
1:M:89:ALA:HB1	2:N:42:HIS:NE2	2.04	0.73
3:R:204:ILE:HG12	3:R:235:MET:CE	2.18	0.73
2:H:20:LYS:HE2	2:H:28:PHE:CD2	2.25	0.71
1:P:29:GLU:CD	2:Q:79:SER:HG	1.96	0.69
1:J:102:GLN:OE1	2:K:91:ARG:NH2	2.23	0.69
1:M:29:GLU:CD	2:N:79:SER:OG	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:29:GLU:CD	2:N:79:SER:HG	1.97	0.68
1:M:20:ASN:HD21	1:M:61:ILE:HA	1.57	0.68
1:D:17:GLN:HE21	1:D:17:GLN:HA	1.58	0.67
2:B:88:VAL:HG12	2:B:88:VAL:O	1.94	0.67
2:E:20:LYS:HE2	2:E:28:PHE:CD2	2.30	0.67
1:A:102:GLN:OE1	2:B:91:ARG:NH2	2.26	0.66
1:P:5:LEU:HB3	1:P:6:PRO:HD2	1.78	0.66
3:F:218:ASN:OD1	3:F:249:LEU:HB2	1.95	0.66
1:A:115:LYS:HA	2:B:88:VAL:HG12	1.77	0.65
1:A:25:TRP:CH2	1:A:73:ARG:HD3	2.31	0.65
1:J:43:SER:HB3	2:K:80:ASP:OD2	1.96	0.65
1:M:49:GLU:O	1:M:53:VAL:HG23	1.96	0.65
2:N:32:GLN:HE21	2:N:32:GLN:CA	2.10	0.65
3:F:282:THR:HG22	3:F:284:GLY:H	1.62	0.65
3:F:322:THR:O	3:F:326:ILE:HG12	1.96	0.64
2:Q:59:LYS:HE3	2:Q:59:LYS:H	1.63	0.64
2:N:88:VAL:CG1	2:N:88:VAL:O	2.46	0.64
3:R:204:ILE:HA	3:R:209:THR:O	1.97	0.64
3:C:231:THR:OG1	3:C:234:GLU:HB2	1.99	0.63
1:A:25:TRP:CZ2	1:A:73:ARG:HD3	2.34	0.63
3:F:349:ALA:O	3:F:352:GLU:HG2	1.98	0.63
1:M:70:ILE:HG22	2:N:78:TRP:HZ3	1.62	0.62
1:G:116:TRP:O	2:H:89:TRP:HA	2.00	0.62
1:G:87:MET:SD	2:H:40:SER:OG	2.55	0.61
3:C:239:THR:O	3:C:242:THR:HG22	2.00	0.61
1:P:20:ASN:HD21	1:P:61:ILE:HA	1.66	0.61
1:A:87:MET:SD	2:B:40:SER:OG	2.55	0.61
1:D:116:TRP:O	2:E:89:TRP:HA	2.00	0.61
3:L:253:PHE:CZ	3:L:292:LEU:HG	2.36	0.60
2:N:63:MET:HB2	2:N:118:PHE:HA	1.83	0.60
1:M:89:ALA:HB1	2:N:42:HIS:CE1	2.37	0.60
1:A:43:SER:CB	2:B:80:ASP:OD2	2.50	0.59
3:R:173:ILE:O	3:R:271:ARG:NH2	2.35	0.59
3:F:204:ILE:HA	3:F:209:THR:O	2.01	0.59
1:G:72:LEU:HD11	2:H:76:TRP:HB3	1.83	0.59
3:C:173:ILE:O	3:C:271:ARG:NH2	2.35	0.59
3:L:239:THR:O	3:L:242:THR:HG22	2.02	0.59
1:P:20:ASN:ND2	1:P:61:ILE:HD12	2.17	0.59
3:C:253:PHE:CZ	3:C:292:LEU:HG	2.38	0.59
1:J:72:LEU:HD11	2:K:76:TRP:HB3	1.85	0.59
3:L:231:THR:OG1	3:L:234:GLU:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:TRP:HA	3:C:245:TYR:CE2	2.38	0.58
3:O:260:ARG:NH2	4:O:403:SO4:O4	2.36	0.58
2:Q:88:VAL:CG1	2:Q:88:VAL:O	2.51	0.58
1:A:31:PHE:O	1:A:35:GLN:HG2	2.04	0.58
3:L:322:THR:O	3:L:326:ILE:HD13	2.03	0.57
1:D:72:LEU:HD11	2:E:76:TRP:HB3	1.86	0.57
3:C:322:THR:O	3:C:326:ILE:HD13	2.03	0.57
3:I:339:ARG:O	3:I:360:GLN:NE2	2.38	0.57
3:O:204:ILE:HA	3:O:209:THR:O	2.04	0.57
3:I:349:ALA:O	3:I:352:GLU:HG2	2.04	0.57
3:O:173:ILE:O	3:O:271:ARG:NH2	2.38	0.57
3:R:199:VAL:HG13	3:R:235:MET:HE3	1.86	0.57
1:M:87:MET:HG3	1:M:89:ALA:H	1.69	0.56
1:M:87:MET:O	1:M:88:SER:HB2	2.05	0.56
2:H:88:VAL:HG12	2:H:88:VAL:O	2.06	0.56
1:J:110:TRP:HA	3:L:245:TYR:CE2	2.40	0.56
1:P:29:GLU:CD	2:Q:79:SER:OG	2.40	0.56
2:Q:63:MET:HB2	2:Q:118:PHE:HA	1.88	0.56
2:N:88:VAL:O	2:N:88:VAL:HG12	2.06	0.56
1:P:52:PHE:CD1	1:P:52:PHE:C	2.79	0.55
1:P:69:TRP:HA	1:P:69:TRP:CE3	2.41	0.55
2:N:32:GLN:CA	2:N:32:GLN:NE2	2.69	0.55
2:E:63:MET:HB2	2:E:118:PHE:HA	1.89	0.55
3:F:361:ILE:O	3:F:362:PHE:O	2.25	0.55
1:M:116:TRP:O	2:N:89:TRP:HA	2.07	0.55
1:P:31:PHE:O	1:P:35:GLN:HG2	2.06	0.55
2:Q:59:LYS:H	2:Q:59:LYS:CE	2.20	0.55
1:P:11:TYR:HB2	1:P:52:PHE:CE2	2.42	0.54
1:P:49:GLU:O	1:P:53:VAL:HG23	2.07	0.54
2:B:88:VAL:O	2:B:88:VAL:CG1	2.55	0.54
1:G:31:PHE:O	1:G:35:GLN:HG2	2.07	0.54
2:E:88:VAL:HG12	2:E:88:VAL:O	2.08	0.54
3:L:218:ASN:ND2	3:L:249:LEU:HD12	2.23	0.54
2:N:13:TYR:CE1	2:N:121:LYS:HG3	2.43	0.54
3:F:344:VAL:HG13	3:F:349:ALA:HB3	1.90	0.54
3:L:362:PHE:CD1	3:L:362:PHE:N	2.76	0.53
1:G:87:MET:O	1:G:88:SER:HB3	2.07	0.53
1:G:24:THR:HG22	1:G:26:ASP:H	1.74	0.53
1:G:97:ASN:O	1:G:100:GLU:HB2	2.08	0.53
1:J:18:ALA:HB1	1:J:61:ILE:HD11	1.91	0.53
1:M:5:LEU:HB3	1:M:6:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HA	2:B:88:VAL:CG1	2.39	0.53
1:D:5:LEU:HB3	1:D:6:PRO:HD2	1.91	0.53
1:D:97:ASN:O	1:D:100:GLU:HB2	2.08	0.53
2:K:3:LEU:HD23	2:K:4:HIS:CE1	2.43	0.53
2:E:61:THR:CG2	2:E:100:VAL:HB	2.39	0.53
1:G:95:ASN:ND2	2:H:105:ILE:O	2.40	0.52
2:Q:61:THR:CG2	2:Q:100:VAL:HB	2.40	0.52
2:E:69:ASN:ND2	2:E:72:LYS:HB2	2.25	0.52
3:F:173:ILE:HD12	3:F:361:ILE:CG2	2.38	0.52
2:Q:13:TYR:CE1	2:Q:121:LYS:HG3	2.45	0.52
2:E:90:LEU:HD12	2:E:90:LEU:C	2.30	0.52
1:M:25:TRP:O	1:M:25:TRP:CE3	2.63	0.52
1:P:87:MET:O	1:P:88:SER:HB2	2.08	0.52
1:M:25:TRP:NE1	1:M:70:ILE:O	2.41	0.52
3:F:198:PHE:CD2	3:F:357:LEU:HD23	2.44	0.52
1:J:87:MET:HG3	1:J:89:ALA:H	1.75	0.52
1:P:132:PRO:O	1:P:133:SER:HB3	2.09	0.52
1:J:31:PHE:O	1:J:35:GLN:HG2	2.10	0.52
1:M:78:GLU:OE1	1:M:78:GLU:N	2.41	0.52
1:M:35:GLN:O	1:M:36:ALA:HB3	2.09	0.51
1:G:3:ASN:N	1:G:3:ASN:ND2	2.57	0.51
1:G:5:LEU:HB3	1:G:6:PRO:HD2	1.92	0.51
2:H:69:ASN:ND2	2:H:72:LYS:HB2	2.25	0.51
1:J:87:MET:O	1:J:88:SER:CB	2.58	0.51
3:C:288:ASP:HB2	3:C:291:MET:HE3	1.92	0.51
2:N:61:THR:CG2	2:N:100:VAL:HB	2.41	0.51
1:A:99:GLY:HA2	1:A:120:ASP:HB2	1.92	0.51
3:I:178:VAL:HA	3:I:214:ILE:O	2.10	0.51
1:M:131:PHE:HD1	1:M:132:PRO:O	1.94	0.51
2:B:22:TRP:CD1	2:B:95:CYS:HB3	2.46	0.51
1:D:31:PHE:O	1:D:35:GLN:HG2	2.11	0.51
3:L:362:PHE:N	3:L:362:PHE:HD1	2.09	0.51
1:M:55:GLN:OE1	3:R:207:THR:HG22	2.10	0.51
1:M:99:GLY:HA2	1:M:120:ASP:HB2	1.92	0.51
1:P:78:GLU:N	1:P:78:GLU:OE1	2.44	0.51
1:A:87:MET:HG3	1:A:89:ALA:H	1.76	0.50
2:H:63:MET:HB2	2:H:118:PHE:HA	1.92	0.50
1:A:86:SER:OG	2:B:26:GLU:OE2	2.29	0.50
2:H:88:VAL:O	2:H:88:VAL:CG1	2.59	0.50
2:K:8:TYR:HB2	2:K:49:PHE:CE2	2.47	0.50
1:M:8:TRP:CZ3	1:M:131:PHE:CE2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:VAL:O	2:E:107:TRP:HA	2.12	0.50
1:M:69:TRP:HA	1:M:69:TRP:CE3	2.45	0.50
1:P:116:TRP:O	2:Q:89:TRP:HA	2.11	0.50
2:H:30:TYR:HA	2:H:36:SER:O	2.12	0.50
1:A:72:LEU:HD11	2:B:76:TRP:HB3	1.93	0.50
1:D:78:GLU:OE2	1:D:78:GLU:N	2.45	0.50
1:A:18:ALA:HB1	1:A:61:ILE:HD11	1.94	0.50
1:G:89:ALA:HB1	2:H:42:HIS:NE2	2.27	0.49
1:J:43:SER:CB	2:K:80:ASP:OD2	2.60	0.49
1:J:89:ALA:HB1	2:K:42:HIS:CE1	2.47	0.49
1:P:89:ALA:HB1	2:Q:42:HIS:NE2	2.26	0.49
1:P:99:GLY:HA2	1:P:120:ASP:HB2	1.93	0.49
3:R:344:VAL:HG13	3:R:349:ALA:HB3	1.93	0.49
3:O:216:TYR:CE2	3:O:252:THR:HA	2.47	0.49
1:D:115:LYS:HA	2:E:88:VAL:HG12	1.94	0.49
1:M:33:THR:HA	1:M:39:GLY:O	2.13	0.49
3:O:218:ASN:ND2	3:O:249:LEU:HD12	2.28	0.49
3:I:330:LYS:O	3:I:333:ALA:HB3	2.12	0.49
3:L:233:GLU:O	3:L:237:VAL:HG23	2.12	0.49
3:F:204:ILE:HB	3:F:232:LYS:HG2	1.95	0.49
1:A:94:VAL:HA	2:B:107:TRP:CZ3	2.48	0.49
1:M:75:ARG:HD2	2:N:77:GLU:OE2	2.13	0.49
2:K:13:TYR:CE1	2:K:121:LYS:HG3	2.48	0.49
2:K:30:TYR:HA	2:K:36:SER:O	2.13	0.49
3:O:180:ASP:HB2	3:O:282:THR:HA	1.95	0.48
1:P:8:TRP:CZ3	1:P:131:PHE:CE2	3.01	0.48
3:I:344:VAL:HG13	3:I:349:ALA:HB3	1.94	0.48
3:L:175:VAL:HB	3:L:211:VAL:HG22	1.95	0.48
3:R:180:ASP:HB2	3:R:282:THR:HA	1.94	0.48
1:M:42:VAL:HG13	1:M:70:ILE:HG23	1.95	0.48
3:F:204:ILE:HB	3:F:232:LYS:CG	2.43	0.48
1:P:94:VAL:HG13	1:P:96:TRP:CD1	2.49	0.48
3:I:198:PHE:CD2	3:I:357:LEU:HD23	2.49	0.48
3:R:216:TYR:CE2	3:R:252:THR:HA	2.48	0.48
2:K:32:GLN:O	2:K:33:HIS:HB2	2.14	0.48
3:C:344:VAL:HG13	3:C:349:ALA:HB3	1.94	0.48
1:G:78:GLU:OE1	1:G:78:GLU:N	2.47	0.48
3:F:339:ARG:O	3:F:360:GLN:NE2	2.47	0.48
1:A:63:ARG:O	1:A:109:ARG:NH2	2.46	0.48
3:L:176:VAL:HA	3:L:212:GLY:O	2.14	0.48
3:R:204:ILE:CG1	3:R:235:MET:HE1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:O	1:A:53:VAL:HG23	2.14	0.47
3:I:357:LEU:O	3:I:361:ILE:HG12	2.13	0.47
1:D:17:GLN:HA	1:D:17:GLN:NE2	2.27	0.47
1:D:87:MET:O	1:D:88:SER:HB3	2.12	0.47
1:D:93:TYR:CE2	1:J:77:LYS:HB2	2.49	0.47
2:H:97:VAL:O	2:H:107:TRP:HA	2.14	0.47
2:N:65:LEU:HD21	2:N:98:MET:HB2	1.94	0.47
3:R:239:THR:O	3:R:242:THR:HG22	2.14	0.47
1:A:75:ARG:HD3	4:A:202:SO4:O3	2.13	0.47
3:C:233:GLU:O	3:C:237:VAL:HG23	2.13	0.47
1:P:11:TYR:HB2	1:P:52:PHE:CD2	2.49	0.47
1:M:75:ARG:CD	2:N:77:GLU:OE2	2.63	0.47
1:D:69:TRP:HB2	1:D:127:PHE:HB3	1.97	0.47
3:L:173:ILE:O	3:L:271:ARG:NH2	2.47	0.47
1:A:25:TRP:CH2	1:A:73:ARG:CD	2.98	0.47
2:H:68:ASN:C	2:H:68:ASN:OD1	2.53	0.47
3:O:173:ILE:O	3:O:209:THR:HA	2.15	0.47
1:A:8:TRP:CZ3	1:A:131:PHE:CE2	3.02	0.47
2:B:36:SER:HA	2:B:121:LYS:O	2.15	0.47
1:P:87:MET:HG3	1:P:89:ALA:H	1.79	0.47
2:Q:30:TYR:HA	2:Q:36:SER:O	2.15	0.46
3:O:231:THR:OG1	3:O:234:GLU:HB2	2.15	0.46
1:P:20:ASN:O	1:P:22:PRO:HD3	2.15	0.46
2:H:92:ARG:HB2	2:H:93:PRO:CD	2.45	0.46
3:L:322:THR:O	3:L:326:ILE:CD1	2.63	0.46
1:D:30:ARG:O	1:D:33:THR:OG1	2.29	0.46
3:O:181:GLU:HG3	3:O:181:GLU:O	2.16	0.46
1:A:75:ARG:HD2	2:B:77:GLU:OE2	2.14	0.46
3:F:178:VAL:HA	3:F:214:ILE:O	2.14	0.46
1:P:33:THR:HA	1:P:39:GLY:O	2.15	0.46
1:P:87:MET:SD	2:Q:40:SER:CB	3.04	0.46
1:J:49:GLU:O	1:J:53:VAL:HG23	2.16	0.46
2:Q:59:LYS:H	2:Q:59:LYS:CD	2.28	0.46
3:F:337:THR:O	3:F:341:PHE:HB3	2.15	0.46
3:I:356:THR:HG22	3:I:360:GLN:OE1	2.15	0.46
2:Q:65:LEU:HD21	2:Q:98:MET:HB2	1.97	0.46
3:F:216:TYR:CD2	3:F:216:TYR:C	2.89	0.46
3:I:361:ILE:O	3:I:362:PHE:O	2.34	0.46
1:J:89:ALA:HB1	2:K:42:HIS:NE2	2.31	0.46
1:G:33:THR:HG22	1:G:39:GLY:O	2.16	0.46
2:E:16:PHE:HB3	2:E:18:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:PHE:O	1:M:35:GLN:HG2	2.17	0.45
3:L:175:VAL:O	3:L:211:VAL:HA	2.15	0.45
3:R:188:TRP:CD2	3:R:244:GLN:HB2	2.52	0.45
2:E:61:THR:HG21	2:E:100:VAL:HB	1.98	0.45
3:F:330:LYS:O	3:F:333:ALA:HB3	2.16	0.45
3:I:204:ILE:HA	3:I:209:THR:O	2.17	0.45
3:R:218:ASN:ND2	3:R:249:LEU:HD12	2.32	0.45
3:C:329:ILE:N	3:C:329:ILE:HD13	2.31	0.45
2:H:107:TRP:N	2:H:107:TRP:CD1	2.85	0.45
1:M:94:VAL:HG13	1:M:96:TRP:CD1	2.52	0.45
2:N:32:GLN:HE21	2:N:32:GLN:N	2.14	0.45
2:E:30:TYR:HA	2:E:36:SER:O	2.17	0.45
1:A:87:MET:SD	2:B:40:SER:CB	3.05	0.45
2:E:88:VAL:O	2:E:88:VAL:CG1	2.64	0.45
1:D:53:VAL:O	1:D:57:VAL:HG23	2.17	0.45
2:E:90:LEU:HD12	2:E:91:ARG:N	2.31	0.45
2:Q:88:VAL:O	2:Q:88:VAL:HG12	2.16	0.45
1:P:25:TRP:NE1	1:P:70:ILE:O	2.49	0.44
2:H:21:THR:HG23	2:H:112:CYS:O	2.16	0.44
3:O:272:ARG:HG3	3:O:273:SER:N	2.33	0.44
2:Q:58:LEU:HA	2:Q:59:LYS:HE3	1.99	0.44
1:A:18:ALA:HB1	1:A:61:ILE:CD1	2.47	0.44
2:E:92:ARG:HB2	2:E:93:PRO:CD	2.47	0.44
2:Q:32:GLN:CA	2:Q:32:GLN:NE2	2.81	0.44
2:N:32:GLN:NE2	2:N:32:GLN:HA	2.31	0.44
1:G:43:SER:HB3	2:H:80:ASP:OD2	2.17	0.44
2:H:36:SER:HA	2:H:121:LYS:O	2.17	0.44
2:K:22:TRP:CD1	2:K:95:CYS:HB3	2.53	0.44
3:C:322:THR:O	3:C:326:ILE:CD1	2.66	0.44
1:D:89:ALA:HB1	2:E:42:HIS:NE2	2.32	0.44
1:M:69:TRP:C	1:M:70:ILE:HG13	2.37	0.44
2:Q:34:LYS:N	2:Q:34:LYS:HD2	2.33	0.44
3:C:335:ILE:HG23	3:O:305:LEU:CD2	2.48	0.44
2:E:1:CYS:SG	2:E:7:SER:HB2	2.57	0.44
2:E:14:ARG:HD3	2:E:16:PHE:CZ	2.53	0.44
3:I:211:VAL:HB	3:I:235:MET:SD	2.58	0.44
1:J:18:ALA:HB1	1:J:61:ILE:CD1	2.47	0.44
2:N:1:CYS:SG	2:N:7:SER:HB3	2.58	0.44
2:E:3:LEU:O	2:E:4:HIS:HB2	2.18	0.44
1:G:53:VAL:O	1:G:57:VAL:HG23	2.18	0.44
1:G:118:TYR:CE2	2:H:71:TRP:CG	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:231:THR:HB	3:I:234:GLU:HB2	2.00	0.44
3:I:292:LEU:C	3:I:292:LEU:HD23	2.38	0.43
2:K:36:SER:HA	2:K:121:LYS:O	2.16	0.43
1:A:87:MET:O	1:A:88:SER:CB	2.67	0.43
3:I:216:TYR:CD2	3:I:216:TYR:C	2.91	0.43
2:N:107:TRP:CD1	2:N:107:TRP:N	2.85	0.43
1:P:73:ARG:NH1	1:P:75:ARG:HA	2.33	0.43
3:C:339:ARG:NH2	7:C:404:CL:CL	2.88	0.43
3:F:173:ILE:HD12	3:F:361:ILE:HG22	1.99	0.43
1:J:94:VAL:HA	2:K:107:TRP:CZ3	2.54	0.43
1:P:67:TYR:HE2	1:P:117:ASP:HB3	1.84	0.43
3:R:204:ILE:HG12	3:R:235:MET:HE2	2.00	0.43
3:F:264:TYR:O	3:F:270:GLY:HA3	2.19	0.43
3:O:239:THR:O	3:O:242:THR:HG22	2.18	0.43
1:G:72:LEU:CD1	2:H:76:TRP:HB3	2.49	0.43
1:G:85:TRP:CG	2:H:40:SER:HB2	2.53	0.43
2:Q:1:CYS:SG	2:Q:7:SER:HB3	2.57	0.43
2:H:90:LEU:HD12	2:H:90:LEU:C	2.38	0.43
2:K:71:TRP:HA	2:K:74:CYS:SG	2.59	0.43
1:M:109:ARG:HA	1:M:113:PHE:CE1	2.54	0.43
1:D:111:THR:HG21	2:E:90:LEU:CD2	2.49	0.43
1:P:68:VAL:HA	1:P:126:PRO:O	2.18	0.43
2:Q:107:TRP:CD1	2:Q:107:TRP:N	2.86	0.43
3:R:283:ASP:HA	3:R:311:VAL:O	2.19	0.43
3:C:218:ASN:ND2	3:C:249:LEU:HD12	2.33	0.42
3:C:283:ASP:HA	3:C:311:VAL:O	2.19	0.42
3:I:296:ILE:O	3:I:299:CYS:HB2	2.19	0.42
1:J:61:ILE:O	1:J:61:ILE:HG22	2.19	0.42
1:M:33:THR:HG22	1:M:39:GLY:O	2.19	0.42
1:M:35:GLN:O	1:M:36:ALA:CB	2.67	0.42
2:B:68:ASN:HA	2:B:95:CYS:SG	2.59	0.42
1:D:42:VAL:HB	1:D:128:VAL:HG12	2.01	0.42
2:H:92:ARG:HB2	2:H:93:PRO:HD2	2.01	0.42
2:N:30:TYR:HA	2:N:36:SER:O	2.19	0.42
2:N:40:SER:O	2:N:41:ILE:HD13	2.20	0.42
1:P:109:ARG:HA	1:P:113:PHE:CE1	2.55	0.42
2:B:30:TYR:HA	2:B:36:SER:O	2.20	0.42
3:F:292:LEU:C	3:F:292:LEU:HD23	2.39	0.42
3:I:195:LEU:CB	3:I:239:THR:CG2	2.97	0.42
1:P:40:HIS:ND1	2:Q:80:ASP:HA	2.35	0.42
1:M:78:GLU:H	1:M:78:GLU:CD	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:344:VAL:HG13	3:O:349:ALA:HB3	2.02	0.42
2:H:69:ASN:HD22	2:H:72:LYS:HB2	1.84	0.42
3:O:188:TRP:CD2	3:O:244:GLN:HB2	2.54	0.42
1:G:115:LYS:HA	2:H:88:VAL:HG12	2.02	0.42
2:N:22:TRP:HD1	2:N:64:TRP:CE3	2.37	0.42
3:O:214:ILE:HD11	3:O:263:ALA:HB2	2.02	0.42
3:C:175:VAL:O	3:C:211:VAL:HA	2.18	0.42
2:E:28:PHE:CE1	2:E:32:GLN:NE2	2.88	0.42
2:H:63:MET:HA	2:H:117:SER:O	2.20	0.42
2:H:90:LEU:HD12	2:H:91:ARG:N	2.34	0.42
1:J:86:SER:OG	2:K:26:GLU:OE2	2.37	0.42
1:M:70:ILE:HD11	1:M:107:LEU:N	2.35	0.42
1:M:87:MET:SD	2:N:40:SER:CB	3.07	0.42
1:D:13:GLN:HE21	1:D:13:GLN:HB2	1.74	0.42
2:E:36:SER:HA	2:E:121:LYS:O	2.18	0.42
3:I:259:ALA:O	3:I:263:ALA:HB3	2.20	0.42
3:L:283:ASP:HA	3:L:311:VAL:O	2.20	0.42
1:M:37:LYS:O	1:M:38:ARG:HB2	2.19	0.42
2:Q:1:CYS:HB3	2:Q:2:PRO:HD2	2.02	0.42
1:A:87:MET:SD	2:B:40:SER:HB3	2.60	0.42
2:K:107:TRP:N	2:K:107:TRP:CD1	2.87	0.42
3:R:305:LEU:HD12	3:R:305:LEU:HA	1.80	0.42
3:I:288:ASP:HB2	3:I:291:MET:HE3	2.02	0.41
1:J:25:TRP:CH2	1:J:73:ARG:HD3	2.55	0.41
2:E:20:LYS:HD2	2:E:118:PHE:HE2	1.86	0.41
3:F:194:PHE:CD1	3:F:350:LEU:HD22	2.55	0.41
1:J:72:LEU:CD1	2:K:76:TRP:HB3	2.50	0.41
1:M:20:ASN:O	1:M:22:PRO:HD3	2.20	0.41
1:M:62:LYS:O	1:M:62:LYS:HG2	2.20	0.41
1:P:56:LEU:O	1:P:56:LEU:HD23	2.19	0.41
3:L:173:ILE:HB	3:L:209:THR:HG22	2.01	0.41
1:A:5:LEU:HB3	1:A:6:PRO:HD2	2.03	0.41
1:D:131:PHE:HD1	1:D:132:PRO:O	2.04	0.41
1:G:30:ARG:O	1:G:33:THR:OG1	2.32	0.41
1:M:20:ASN:OD1	1:M:62:LYS:N	2.51	0.41
1:M:68:VAL:HA	1:M:126:PRO:O	2.21	0.41
2:K:63:MET:HB2	2:K:118:PHE:HA	2.03	0.41
2:K:116:VAL:C	2:K:117:SER:O	2.58	0.41
3:O:242:THR:O	3:O:242:THR:HG23	2.21	0.41
1:A:63:ARG:HB3	1:A:65:GLU:OE1	2.21	0.41
1:P:74:ASP:OD2	2:Q:75:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:131:PHE:HD1	1:P:132:PRO:O	2.03	0.41
1:D:109:ARG:HA	1:D:113:PHE:CE1	2.55	0.41
3:F:211:VAL:HB	3:F:235:MET:SD	2.60	0.41
1:G:3:ASN:N	1:G:3:ASN:HD22	2.19	0.41
3:L:199:VAL:HA	3:L:202:LEU:HD12	2.01	0.41
2:B:32:GLN:O	2:B:33:HIS:HB2	2.20	0.41
2:E:63:MET:HA	2:E:117:SER:O	2.21	0.41
3:F:283:ASP:HA	3:F:311:VAL:O	2.21	0.41
1:G:85:TRP:HE3	2:H:66:GLY:O	2.04	0.41
3:L:216:TYR:CE2	3:L:252:THR:HA	2.55	0.41
2:N:20:LYS:O	2:N:115:THR:HA	2.21	0.41
3:C:173:ILE:HD12	3:C:209:THR:HG22	2.03	0.41
1:D:39:GLY:O	1:D:40:HIS:CD2	2.74	0.41
1:J:110:TRP:CG	3:L:247:GLY:HA2	2.56	0.41
2:Q:116:VAL:C	2:Q:117:SER:O	2.58	0.41
3:C:188:TRP:CD2	3:C:244:GLN:HB2	2.56	0.40
2:E:86:TYR:CZ	2:E:88:VAL:HG21	2.56	0.40
3:I:264:TYR:O	3:I:270:GLY:HA3	2.21	0.40
3:R:322:THR:O	3:R:323:LYS:C	2.60	0.40
1:A:86:SER:N	2:B:66:GLY:O	2.42	0.40
1:P:35:GLN:O	1:P:36:ALA:HB2	2.21	0.40
2:B:107:TRP:N	2:B:107:TRP:CD1	2.88	0.40
2:E:14:ARG:HG2	2:E:16:PHE:CE1	2.56	0.40
3:F:356:THR:HG22	3:F:360:GLN:OE1	2.21	0.40
1:A:116:TRP:O	2:B:89:TRP:HA	2.21	0.40
2:K:118:PHE:CD1	2:K:118:PHE:N	2.90	0.40
3:I:180:ASP:CB	3:I:282:THR:HA	2.51	0.40
2:K:21:THR:HA	2:K:114:LYS:O	2.22	0.40
2:N:116:VAL:C	2:N:117:SER:O	2.59	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	129/135 (96%)	113 (88%)	15 (12%)	1 (1%)	19	51
1	D	129/135 (96%)	118 (92%)	10 (8%)	1 (1%)	19	51
1	G	129/135 (96%)	116 (90%)	12 (9%)	1 (1%)	19	51
1	J	129/135 (96%)	117 (91%)	11 (8%)	1 (1%)	19	51
1	M	129/135 (96%)	119 (92%)	7 (5%)	3 (2%)	6	23
1	P	129/135 (96%)	114 (88%)	14 (11%)	1 (1%)	19	51
2	B	120/124 (97%)	109 (91%)	7 (6%)	4 (3%)	4	15
2	E	120/124 (97%)	110 (92%)	8 (7%)	2 (2%)	9	31
2	H	120/124 (97%)	111 (92%)	7 (6%)	2 (2%)	9	31
2	K	120/124 (97%)	110 (92%)	7 (6%)	3 (2%)	5	21
2	N	120/124 (97%)	105 (88%)	12 (10%)	3 (2%)	5	21
2	Q	120/124 (97%)	105 (88%)	12 (10%)	3 (2%)	5	21
3	C	189/217 (87%)	179 (95%)	9 (5%)	1 (0%)	29	61
3	F	189/217 (87%)	177 (94%)	12 (6%)	0	100	100
3	I	189/217 (87%)	179 (95%)	10 (5%)	0	100	100
3	L	189/217 (87%)	175 (93%)	12 (6%)	2 (1%)	14	42
3	O	189/217 (87%)	174 (92%)	13 (7%)	2 (1%)	14	42
3	R	189/217 (87%)	176 (93%)	11 (6%)	2 (1%)	14	42
All	All	2628/2856 (92%)	2407 (92%)	189 (7%)	32 (1%)	13	40

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	88	SER
2	E	2	PRO
1	G	88	SER
2	H	2	PRO
2	N	2	PRO
2	Q	3	LEU
2	Q	117	SER
2	B	33	HIS
2	K	3	LEU
2	K	33	HIS
1	M	36	ALA
1	M	41	LEU
1	M	76	ARG
2	N	117	SER

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Mol	Chain	Res	Type
2	H	4	HIS
1	J	88	SER
2	K	117	SER
3	O	217	ALA
3	O	323	LYS
1	P	76	ARG
2	Q	2	PRO
3	R	217	ALA
1	A	88	SER
2	B	117	SER
2	E	4	HIS
3	L	217	ALA
3	L	313	GLY
2	B	9	ASN
2	N	33	HIS
3	R	323	LYS
3	C	217	ALA
2	B	2	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	114/118 (97%)	111 (97%)	3 (3%)	46	77
1	D	114/118 (97%)	108 (95%)	6 (5%)	22	54
1	G	114/118 (97%)	108 (95%)	6 (5%)	22	54
1	J	114/118 (97%)	111 (97%)	3 (3%)	46	77
1	M	114/118 (97%)	109 (96%)	5 (4%)	28	61
1	P	114/118 (97%)	112 (98%)	2 (2%)	59	85
2	B	110/112 (98%)	103 (94%)	7 (6%)	17	45
2	E	110/112 (98%)	103 (94%)	7 (6%)	17	45
2	H	110/112 (98%)	107 (97%)	3 (3%)	44	77
2	K	110/112 (98%)	102 (93%)	8 (7%)	14	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	110/112 (98%)	105 (96%)	5 (4%)	27	61
2	Q	110/112 (98%)	104 (94%)	6 (6%)	21	53
3	C	160/181 (88%)	152 (95%)	8 (5%)	24	57
3	F	160/181 (88%)	154 (96%)	6 (4%)	33	67
3	I	160/181 (88%)	153 (96%)	7 (4%)	28	61
3	L	160/181 (88%)	153 (96%)	7 (4%)	28	61
3	O	160/181 (88%)	157 (98%)	3 (2%)	57	84
3	R	160/181 (88%)	157 (98%)	3 (2%)	57	84
All	All	2304/2466 (93%)	2209 (96%)	95 (4%)	30	64

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	90	SER
1	A	119	SER
2	B	34	LYS
2	B	44	ARG
2	B	55	SER
2	B	67	LEU
2	B	81	ASP
2	B	91	ARG
2	B	122	PHE
3	C	172	LEU
3	C	184	SER
3	C	273	SER
3	C	303	ASN
3	C	339	ARG
3	C	343	ASN
3	C	345	SER
3	C	362	PHE
1	D	13	GLN
1	D	30	ARG
1	D	37	LYS
1	D	78	GLU
1	D	116	TRP
1	D	119	SER
2	E	7	SER
2	E	55	SER

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Mol	Chain	Res	Type
2	E	61	THR
2	E	67	LEU
2	E	81	ASP
2	E	102	THR
2	E	122	PHE
3	F	184	SER
3	F	207	THR
3	F	231	THR
3	F	321	ASP
3	F	334	SER
3	F	345	SER
1	G	3	ASN
1	G	30	ARG
1	G	84	GLU
1	G	116	TRP
1	G	118	TYR
1	G	119	SER
2	H	55	SER
2	H	81	ASP
2	H	122	PHE
3	I	184	SER
3	I	206	PRO
3	I	231	THR
3	I	282	THR
3	I	283	ASP
3	I	321	ASP
3	I	345	SER
1	J	3	ASN
1	J	90	SER
1	J	119	SER
2	K	37	ARG
2	K	45	GLU
2	K	55	SER
2	K	79	SER
2	K	81	ASP
2	K	91	ARG
2	K	110	ARG
2	K	122	PHE
3	L	273	SER
3	L	303	ASN
3	L	321	ASP
3	L	334	SER

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Mol	Chain	Res	Type
3	L	343	ASN
3	L	345	SER
3	L	362	PHE
1	M	3	ASN
1	M	20	ASN
1	M	35	GLN
1	M	47	ASP
1	M	88	SER
2	N	32	GLN
2	N	55	SER
2	N	63	MET
2	N	91	ARG
2	N	122	PHE
3	O	283	ASP
3	O	286	SER
3	O	321	ASP
1	P	88	SER
1	P	119	SER
2	Q	32	GLN
2	Q	34	LYS
2	Q	55	SER
2	Q	59	LYS
2	Q	91	ARG
2	Q	122	PHE
3	R	283	ASP
3	R	286	SER
3	R	321	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	32	GLN
3	C	200	GLN
1	D	13	GLN
2	E	69	ASN
3	F	303	ASN
1	G	60	ASN
2	H	69	ASN
3	I	303	ASN
1	M	60	ASN
2	N	32	GLN
3	O	241	GLN

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Mol	Chain	Res	Type
3	O	303	ASN
2	Q	32	GLN
3	R	241	GLN

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)

Of 37 ligands modelled in this entry, 21 are monoatomic and 1 is modelled with single atom - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	E	201	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	Q	202	5,6	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	B	201	5,6	4,4,4	0.33	0	6,6,6	0.29	0
4	SO4	A	202	-	4,4,4	0.36	0	6,6,6	0.08	0
4	SO4	J	201	-	4,4,4	0.31	0	6,6,6	0.10	0
4	SO4	E	203	5,6	4,4,4	0.17	0	6,6,6	0.43	0
4	SO4	R	402	-	4,4,4	0.37	0	6,6,6	0.14	0
4	SO4	A	201	-	4,4,4	0.30	0	6,6,6	0.06	0
4	SO4	Q	201	-	4,4,4	0.36	0	6,6,6	0.09	0
4	SO4	O	403	-	4,4,4	0.35	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	G	201	-	4,4,4	0.32	0	6,6,6	0.19	0
4	SO4	N	201	5,6	4,4,4	0.33	0	6,6,6	0.10	0
4	SO4	K	202	6	4,4,4	0.25	0	6,6,6	0.25	0
4	SO4	D	201	-	4,4,4	0.33	0	6,6,6	0.15	0
4	SO4	H	202	5,6	4,4,4	0.27	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

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
4	A	202	SO4	1	0
4	O	403	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	131/135 (97%)	0.12	0	100	100	34, 48, 75, 83	0
1	D	131/135 (97%)	0.07	0	100	100	25, 45, 71, 89	0
1	G	131/135 (97%)	0.06	0	100	100	26, 45, 75, 87	0
1	J	131/135 (97%)	0.10	0	100	100	33, 47, 72, 82	0
1	M	131/135 (97%)	0.50	4 (3%)	49	44	33, 60, 105, 115	0
1	P	131/135 (97%)	0.44	3 (2%)	60	58	33, 59, 106, 124	0
2	B	122/124 (98%)	0.28	2 (1%)	72	71	35, 58, 85, 104	0
2	E	122/124 (98%)	0.28	0	100	100	29, 52, 81, 106	0
2	H	122/124 (98%)	0.25	0	100	100	30, 50, 81, 103	0
2	K	122/124 (98%)	0.32	3 (2%)	57	55	36, 56, 83, 108	0
2	N	122/124 (98%)	0.38	4 (3%)	46	41	33, 57, 86, 119	0
2	Q	122/124 (98%)	0.40	6 (4%)	29	26	34, 57, 87, 112	0
3	C	191/217 (88%)	0.22	1 (0%)	91	91	26, 52, 78, 128	0
3	F	191/217 (88%)	0.21	2 (1%)	82	82	30, 48, 78, 95	0
3	I	191/217 (88%)	0.22	2 (1%)	82	82	29, 47, 75, 104	0
3	L	191/217 (88%)	0.25	3 (1%)	72	71	28, 52, 78, 116	0
3	O	191/217 (88%)	0.25	1 (0%)	91	91	33, 49, 78, 106	0
3	R	191/217 (88%)	0.29	1 (0%)	91	91	29, 48, 76, 109	0
All	All	2664/2856 (93%)	0.25	32 (1%)	79	79	25, 51, 83, 128	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	133	SER	4.0
1	M	12	ASP	3.8
3	L	272	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	40	HIS	2.9
1	P	6	PRO	2.8
2	B	13	TYR	2.6
2	Q	16	PHE	2.6
3	C	272	ARG	2.5
3	I	340	TYR	2.5
2	N	85	ASP	2.4
2	B	5	TRP	2.4
2	Q	85	ASP	2.4
3	L	342	PHE	2.3
1	P	12	ASP	2.2
2	K	5	TRP	2.2
2	N	16	PHE	2.2
2	Q	58	LEU	2.2
2	N	15	VAL	2.2
1	M	133	SER	2.2
3	F	357	LEU	2.2
3	R	339	ARG	2.1
1	M	39	GLY	2.1
3	O	305	LEU	2.1
2	K	119	VAL	2.1
2	Q	65	LEU	2.1
3	I	198	PHE	2.1
3	L	172	LEU	2.1
2	N	6	SER	2.0
2	Q	15	VAL	2.0
2	K	13	TYR	2.0
3	F	172	LEU	2.0
2	Q	59	LYS	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
7	CL	J	202	1/1	0.50	0.21	85,85,85,85	0
7	CL	L	403	1/1	0.69	0.21	67,67,67,67	0
4	SO4	A	202	5/5	0.73	0.24	112,142,155,168	0
7	CL	C	403	1/1	0.74	0.11	72,72,72,72	0
7	CL	H	201	1/1	0.82	0.22	59,59,59,59	0
4	SO4	H	202	5/5	0.83	0.18	43,54,82,91	0
4	SO4	E	203	5/5	0.85	0.19	38,47,73,81	0
8	NH4	D	202	1/1	0.85	0.20	22,22,22,22	0
4	SO4	R	402	5/5	0.86	0.23	67,76,84,90	5
4	SO4	B	201	5/5	0.86	0.18	61,65,95,97	0
4	SO4	N	201	5/5	0.86	0.13	92,100,118,121	0
4	SO4	Q	202	5/5	0.87	0.18	104,113,124,133	0
7	CL	E	202	1/1	0.88	0.13	50,50,50,50	0
4	SO4	O	403	5/5	0.89	0.10	87,94,107,107	0
4	SO4	K	202	5/5	0.90	0.15	60,65,89,92	0
6	NA	F	402	1/1	0.90	0.11	26,26,26,26	0
7	CL	K	201	1/1	0.92	0.12	52,52,52,52	0
5	BA	R	401	1/1	0.92	0.10	176,176,176,176	0
7	CL	M	201	1/1	0.92	0.07	54,54,54,54	0
6	NA	L	402	1/1	0.92	0.08	29,29,29,29	0
6	NA	I	402	1/1	0.93	0.09	28,28,28,28	0
7	CL	R	403	1/1	0.93	0.09	53,53,53,53	0
4	SO4	J	201	5/5	0.93	0.11	60,68,70,78	0
5	BA	C	401	1/1	0.94	0.09	132,132,132,132	0
4	SO4	E	201	5/5	0.95	0.13	61,70,76,79	0
4	SO4	A	201	5/5	0.95	0.10	60,65,73,81	0
4	SO4	G	201	5/5	0.95	0.14	43,49,53,61	0
4	SO4	D	201	5/5	0.96	0.16	41,47,56,58	0
5	BA	O	401	1/1	0.96	0.10	169,169,169,169	0
4	SO4	Q	201	5/5	0.96	0.13	57,67,71,74	0
6	NA	C	402	1/1	0.96	0.15	25,25,25,25	0
6	NA	R	404	1/1	0.97	0.10	48,48,48,48	0
6	NA	O	402	1/1	0.97	0.10	47,47,47,47	0
5	BA	F	401	1/1	0.98	0.08	99,99,99,99	0
5	BA	I	401	1/1	0.98	0.09	100,100,100,100	0
5	BA	L	401	1/1	0.98	0.08	127,127,127,127	0
7	CL	C	404	1/1	0.98	0.06	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.